

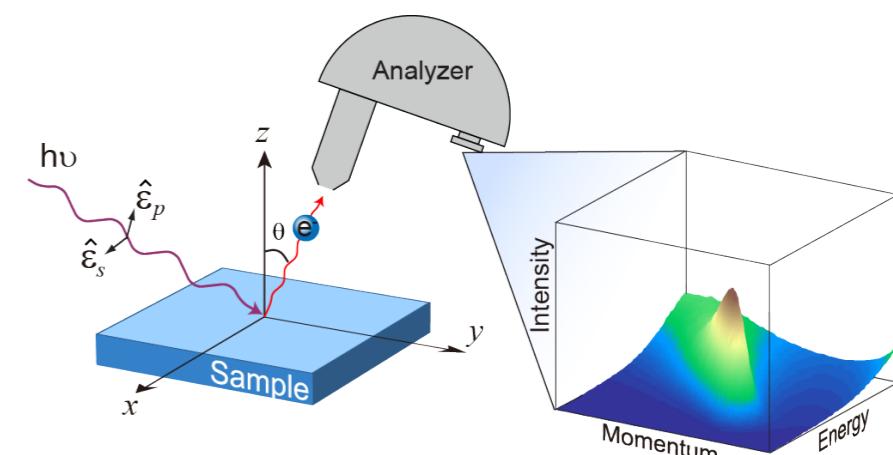
Recent Developments in Fe-based High-temperature Superconductors

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Governing factors of the superconductivity in iron based superconductors: an ARPES study

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Materials:

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- OMBE: Bruce A. Davidson, D. W. Shen, X. F. Zhai
- Z. R. Ye, J. Jiang, X. P. Shen (**Fudan University**)
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Outline

Introduction

What governs the superconductivity in Fe-HTS's

Type 1: Systems with both electron and hole pockets

Type 2: Systems with only electron pockets

Summarize current understanding and future outlook

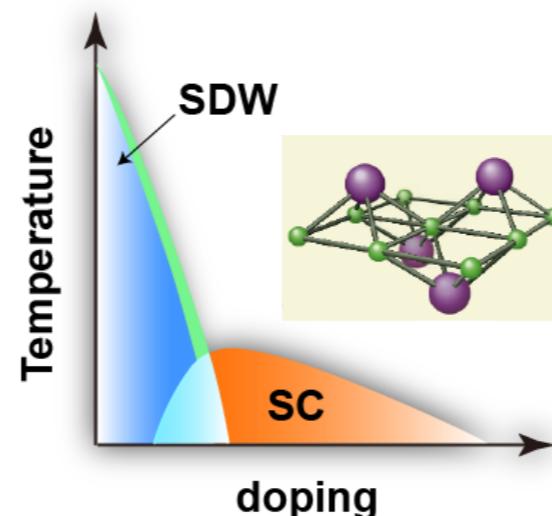
Two types of iron-based superconductors

Fe-HTS's

Type I

Iron pnictides: 11, 111, 122, 1111 series

Maximum Tc: 55K



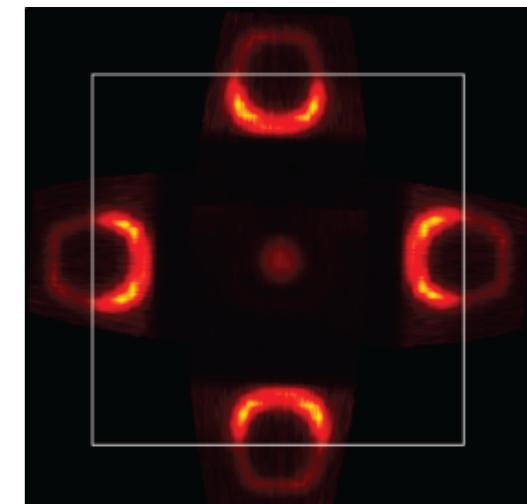
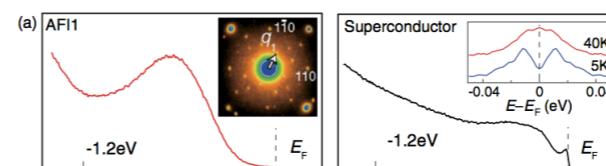
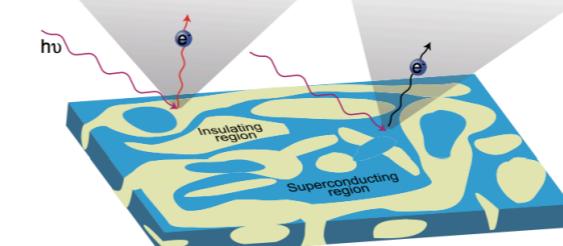
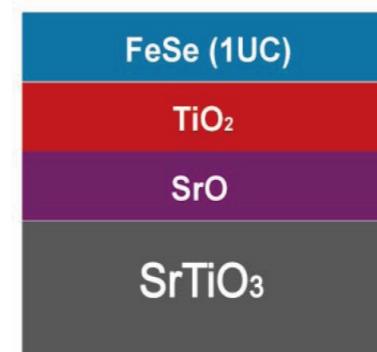
KFe₂Se₂:

Tc: 31K

Type II

1ML FeSe thin film:

Maximum Tc: 65K



What governs T_c ?

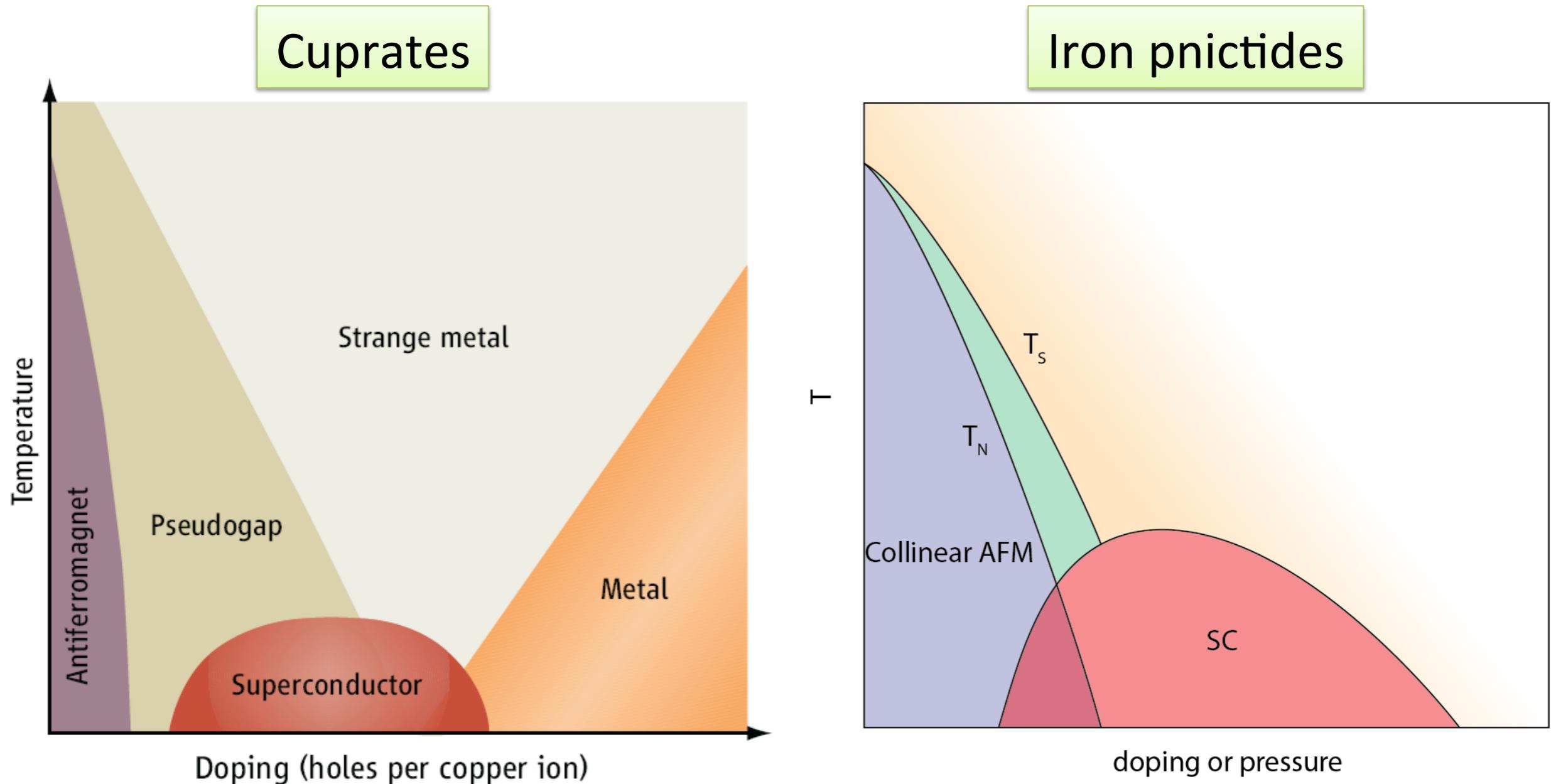
1.

Systems with both electron and hole pockets

2.

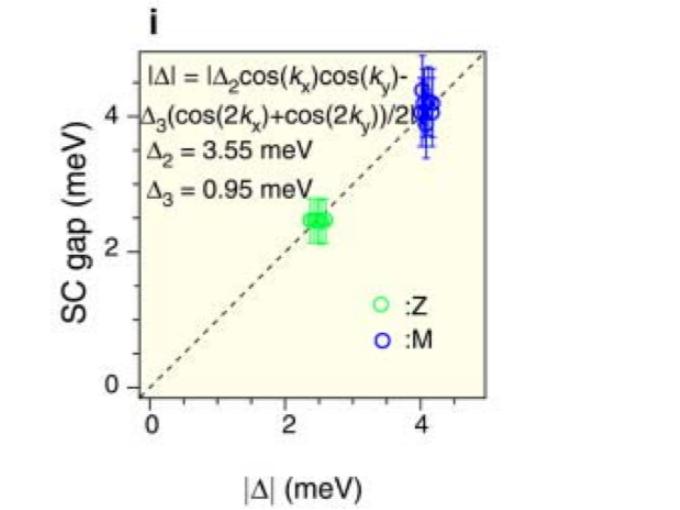
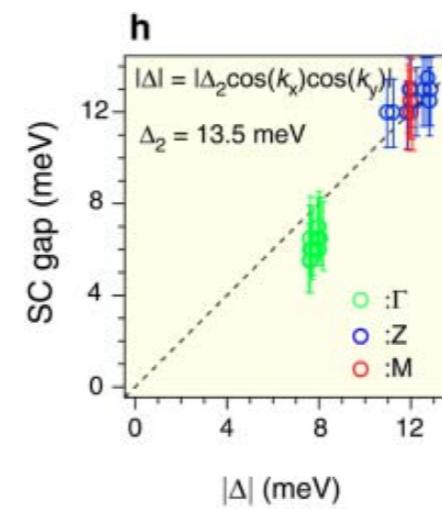
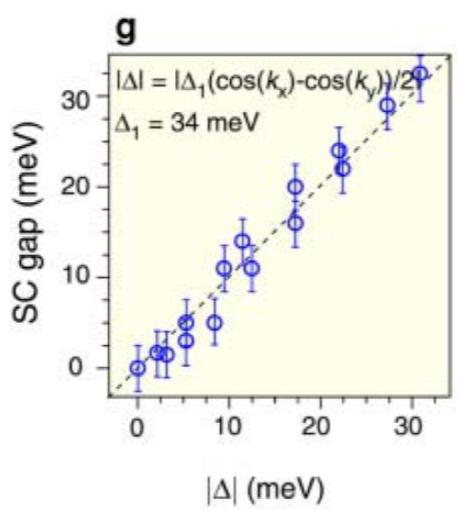
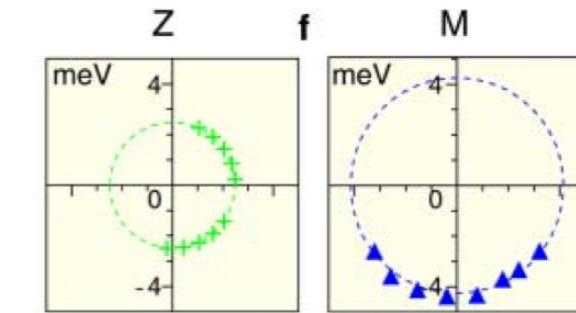
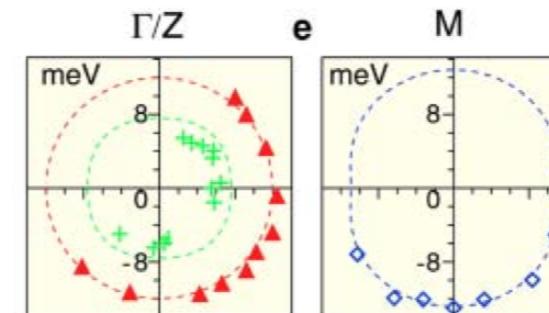
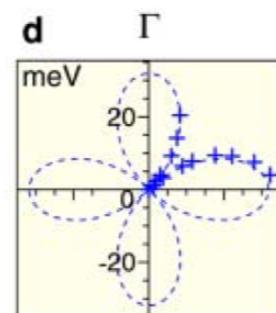
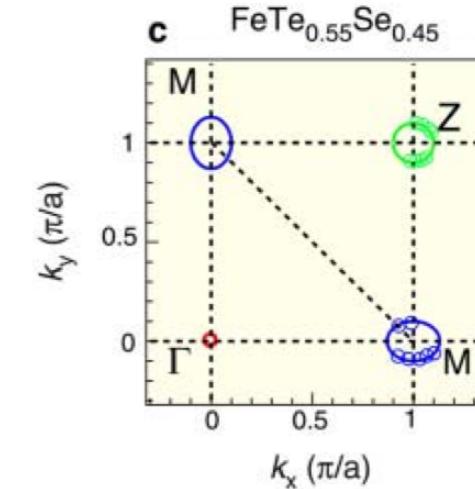
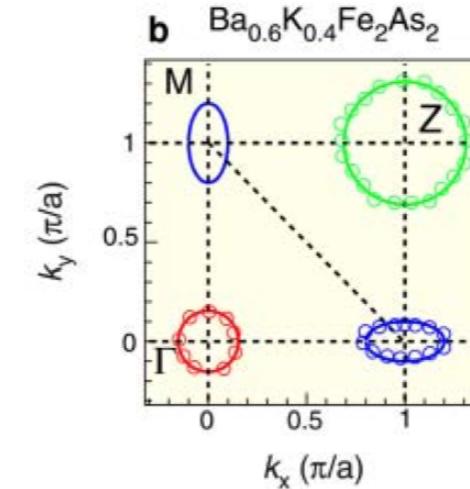
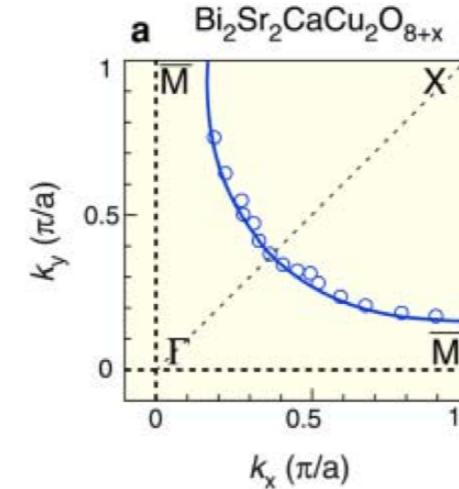
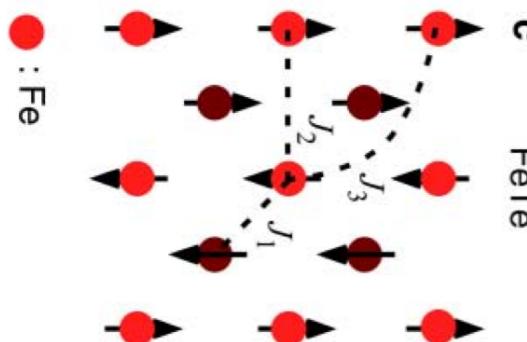
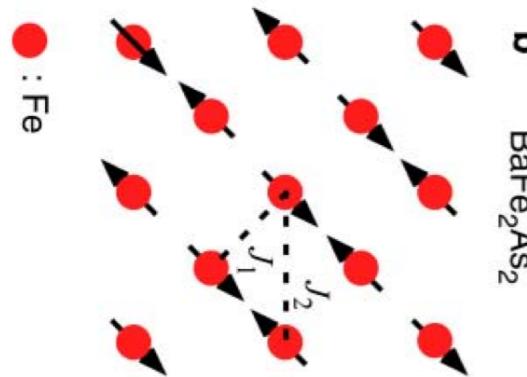
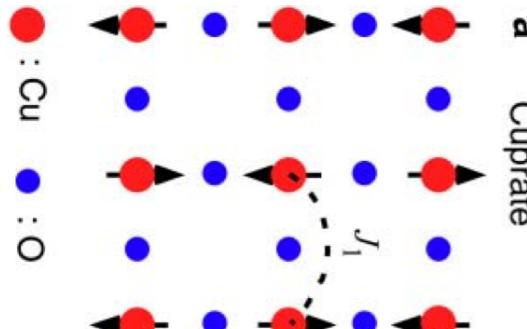
Systems with only electron pockets

Proximity to magnetism

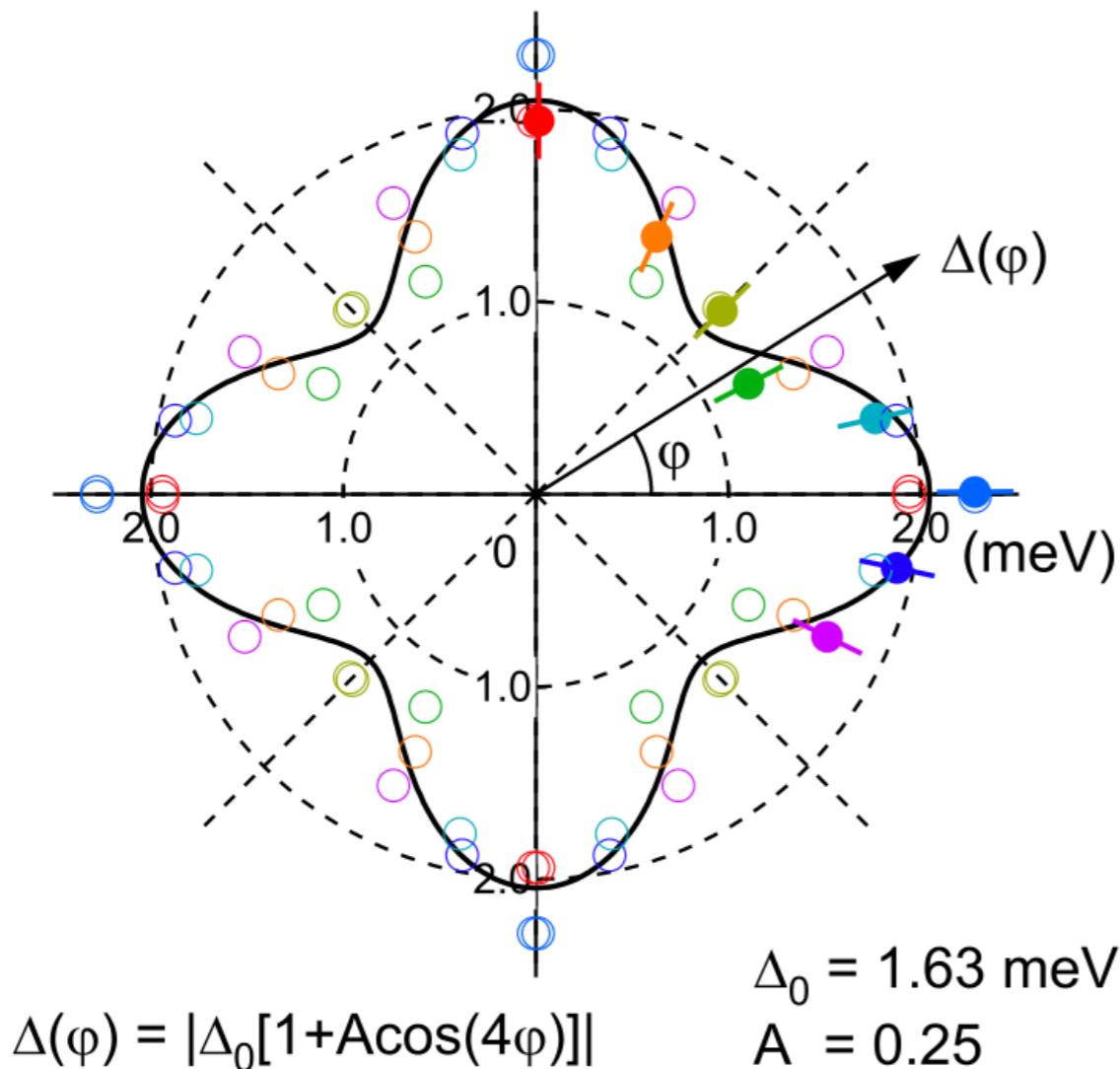


Superconductivity in both cuprates and iron-based superconductors is closely related to magnetism → Unconventional superconductivity with a particular pairing symmetry
spin fluctuations are likely to be the glue.

Universal J_1 - J_2 - J_3 scheme summarized by Hu and Ding



$\cos(4\phi)$ modulation of the superconducting gap of optimally doped $\text{FeTe}_{0.6}\text{Se}_{0.4}$

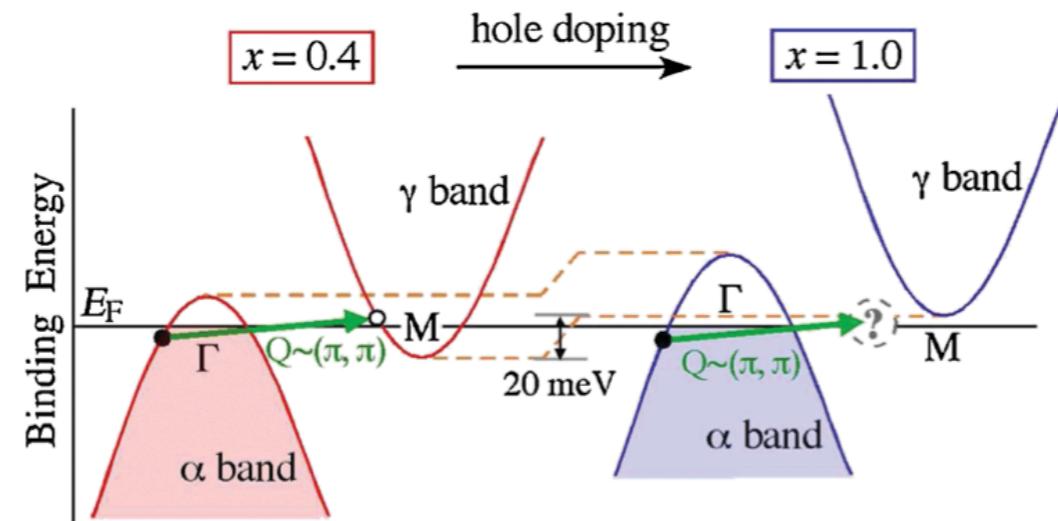
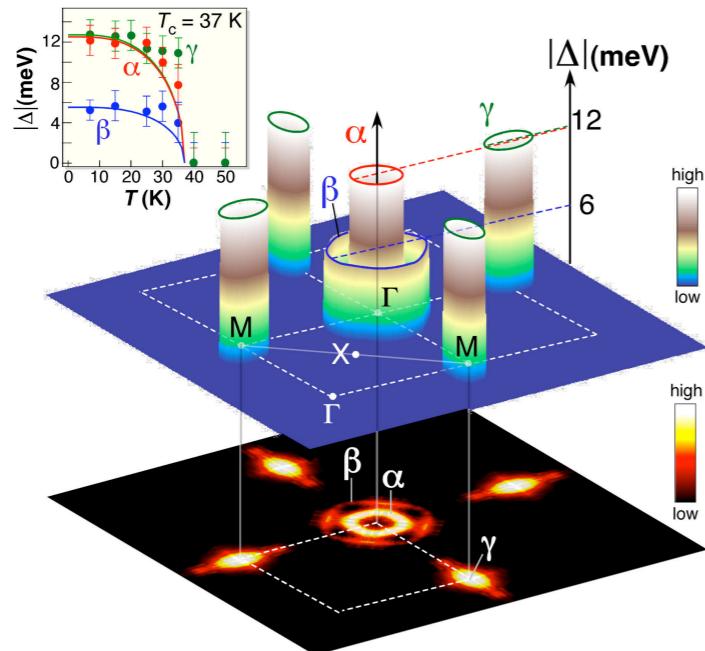


anisotropy in the hole pocket
also suggest the role of J_3

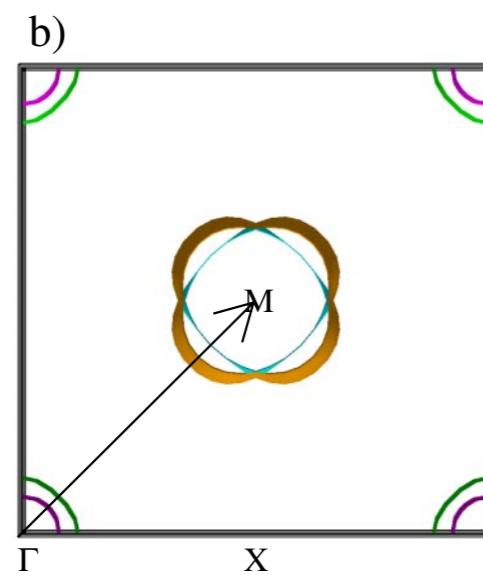
Okazaki, shin et al. arxiv.org/pdf/1207.6571.pdf

- The predicted gaps functions qualitatively fit the measured.
- Quantitative correlation between T_c and J 's is lacking.
- Refinements are necessary, when there are complexities such as k_z dependence, impurity, nodes, SDW ...

Fermi surface nesting ?

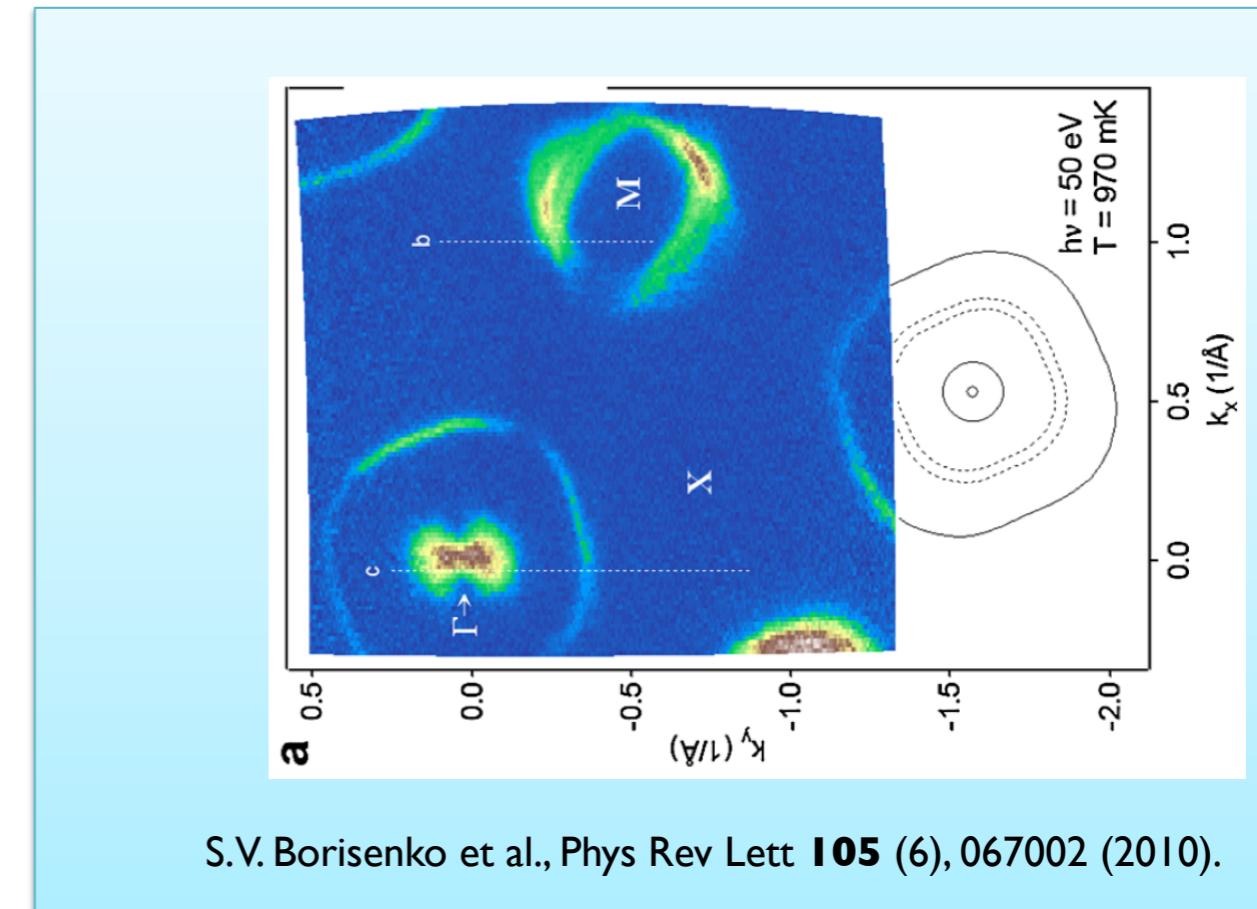


T. Sato et al., Phys Rev Lett **103** 047002 (2009).



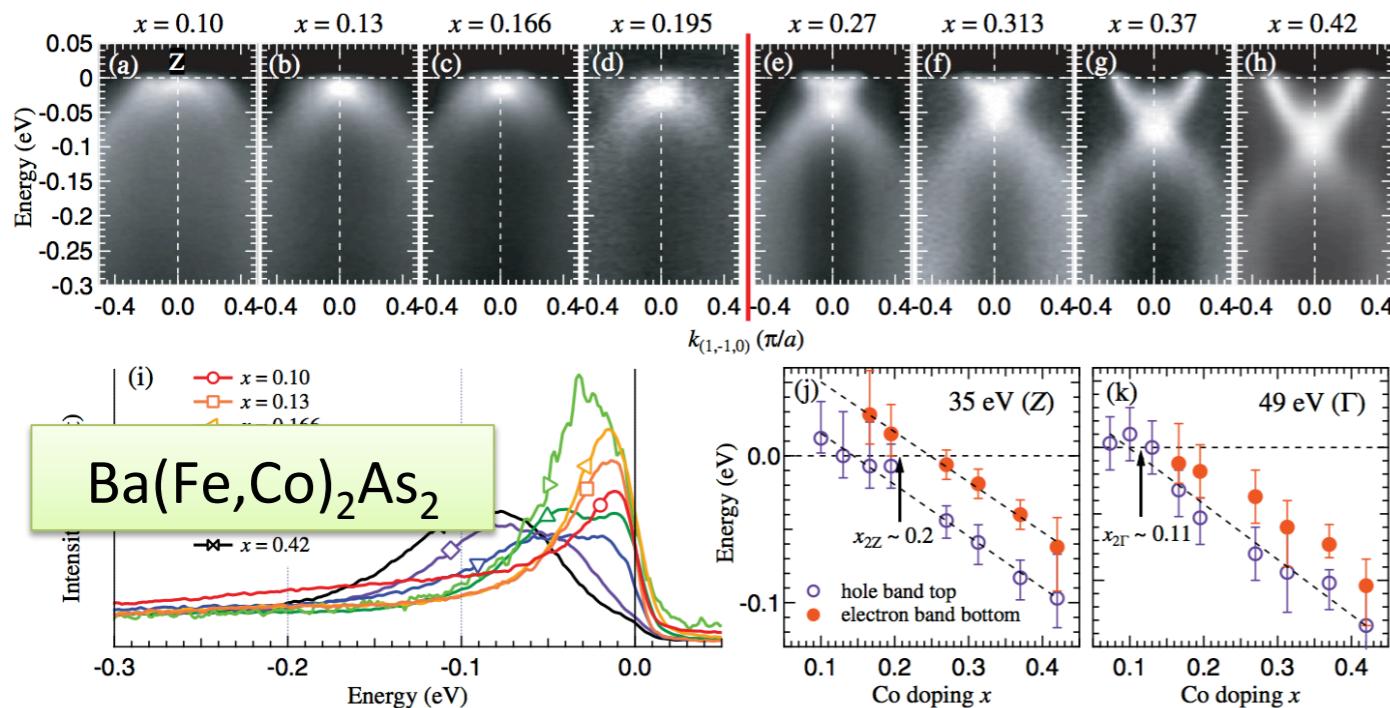
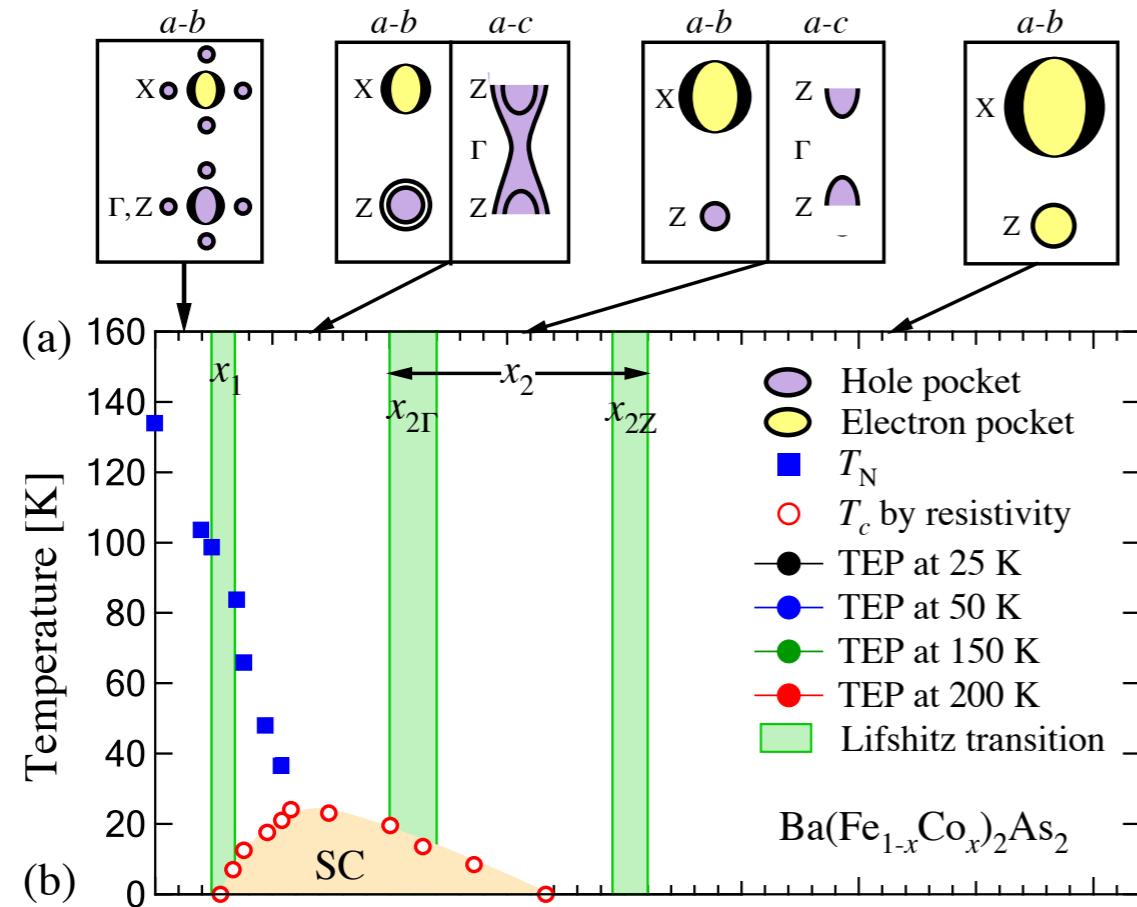
H. Ding et al., EPL **83** (4), 47001 (2008).

I. I. Mazin Phys Rev Lett **101** (5), 057003 (2008).



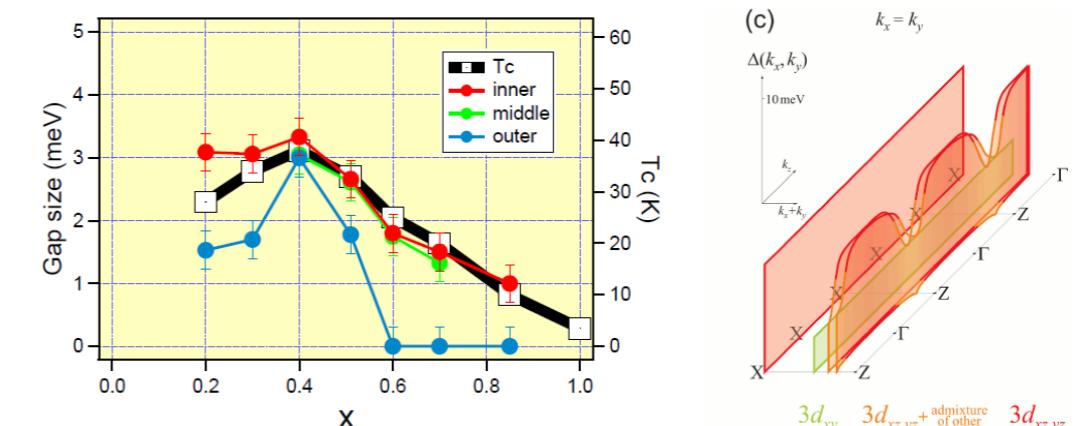
S.V. Borisenko et al., Phys Rev Lett **105** (6), 067002 (2010).

Lifshitz transition ?



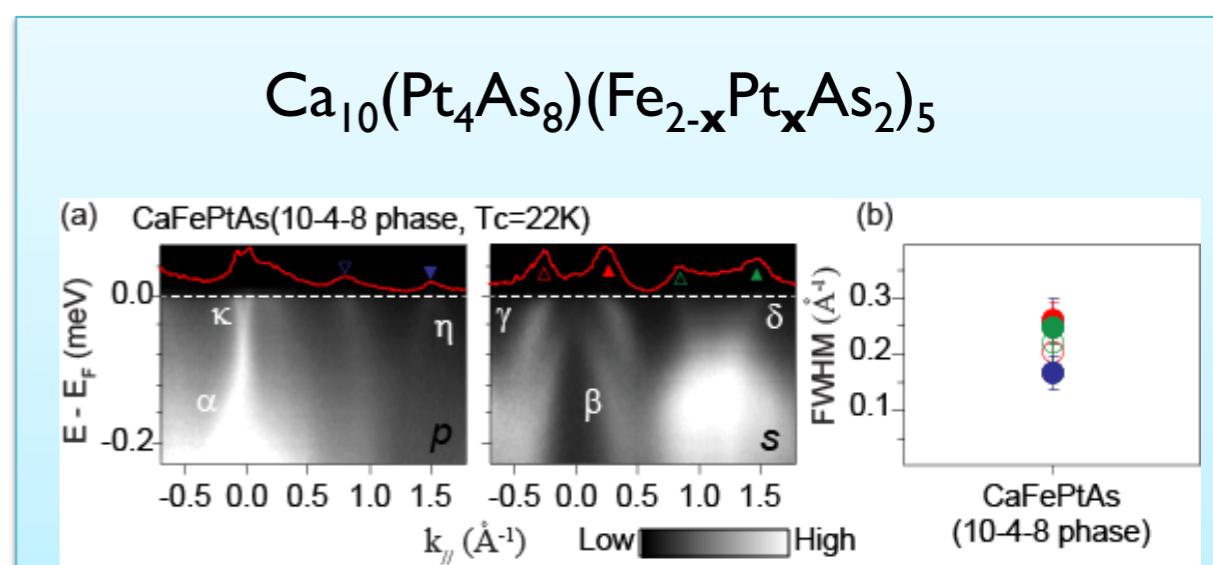
C. Liu et al., Phys Rev B 84 (2), 020509 (2011).

Leading role of dxz/dyz



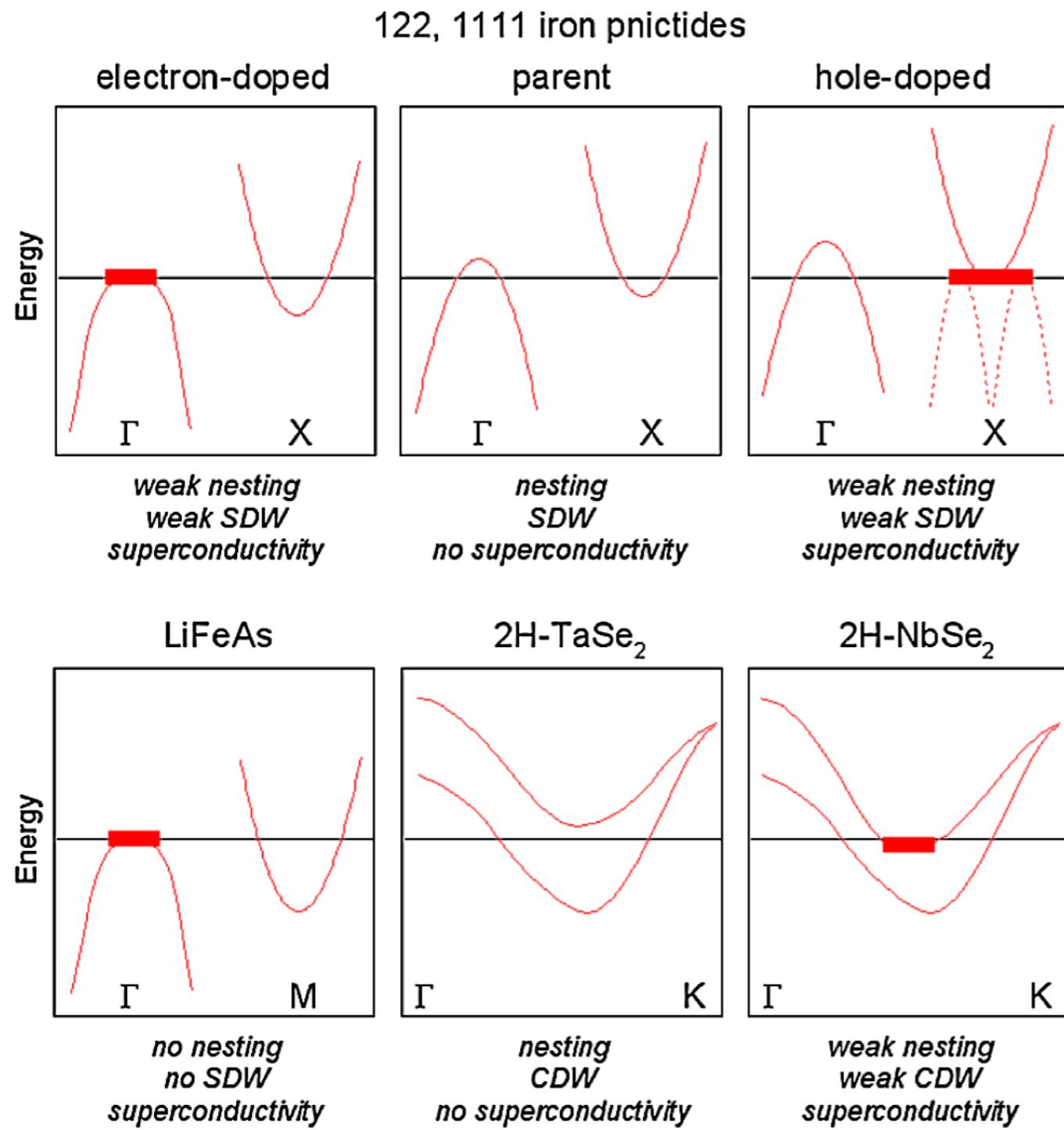
W. Malaeb et al., Phys. Rev. B 86, 165117 (2012)
D.V. Evtushinsky et al., arXiv, 1204.2432 (2012).

Tc diminishes around the Lifshitz transition of dxz/dyz hole pockets

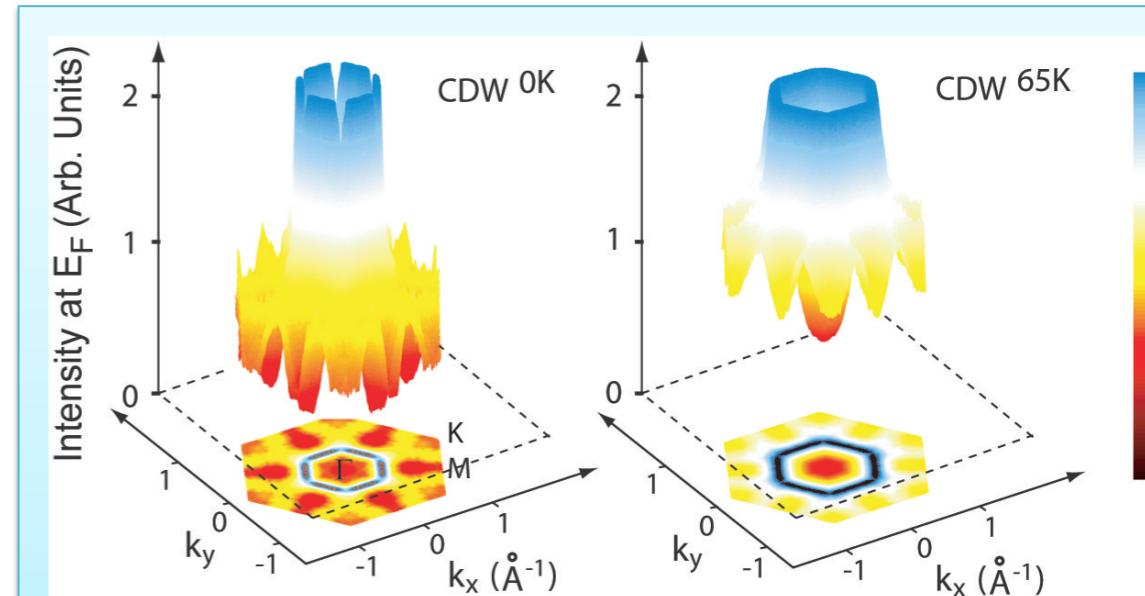
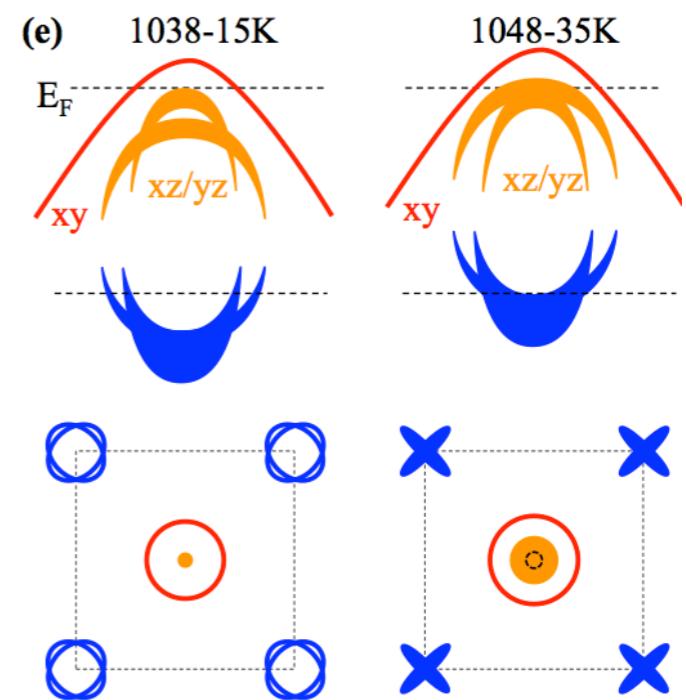


$T_c \sim 22 \text{ K}$, with only dxy hole Fermi surface,
Umm?

van Hove singularity ?



CaFePtAs system



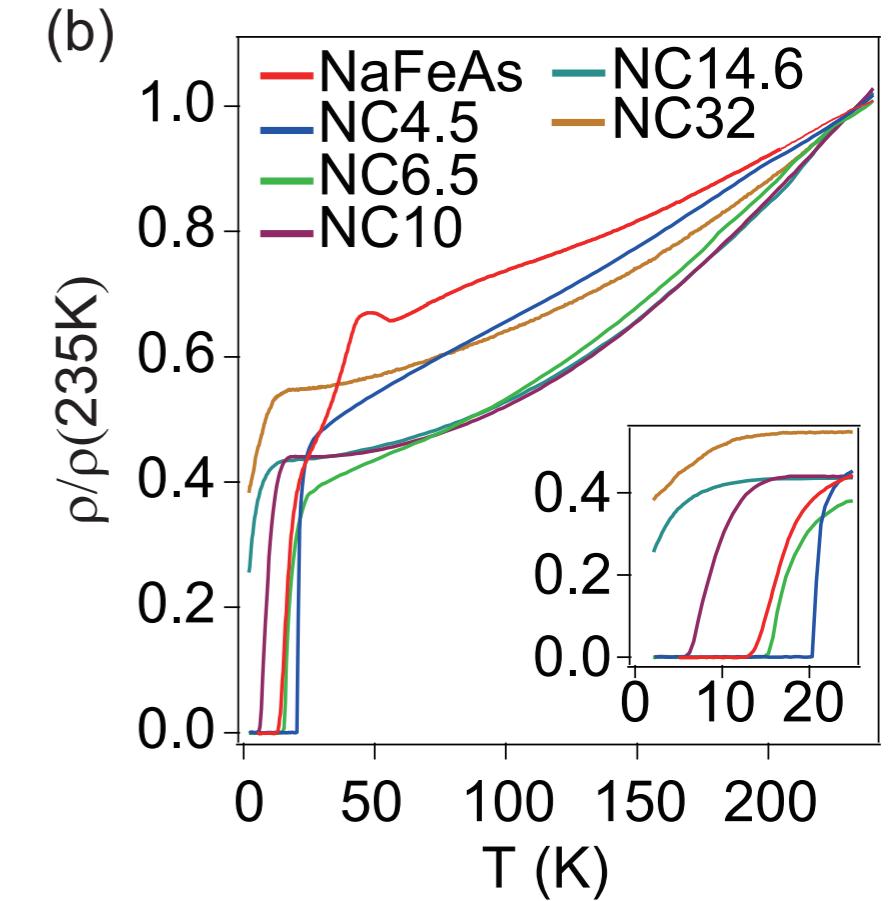
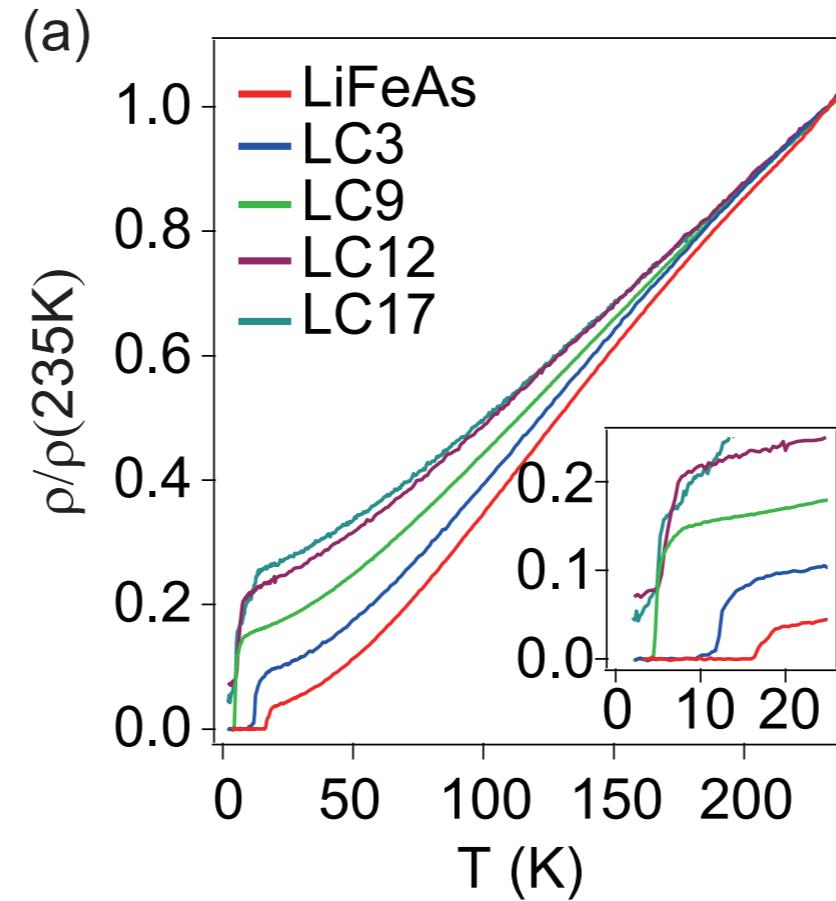
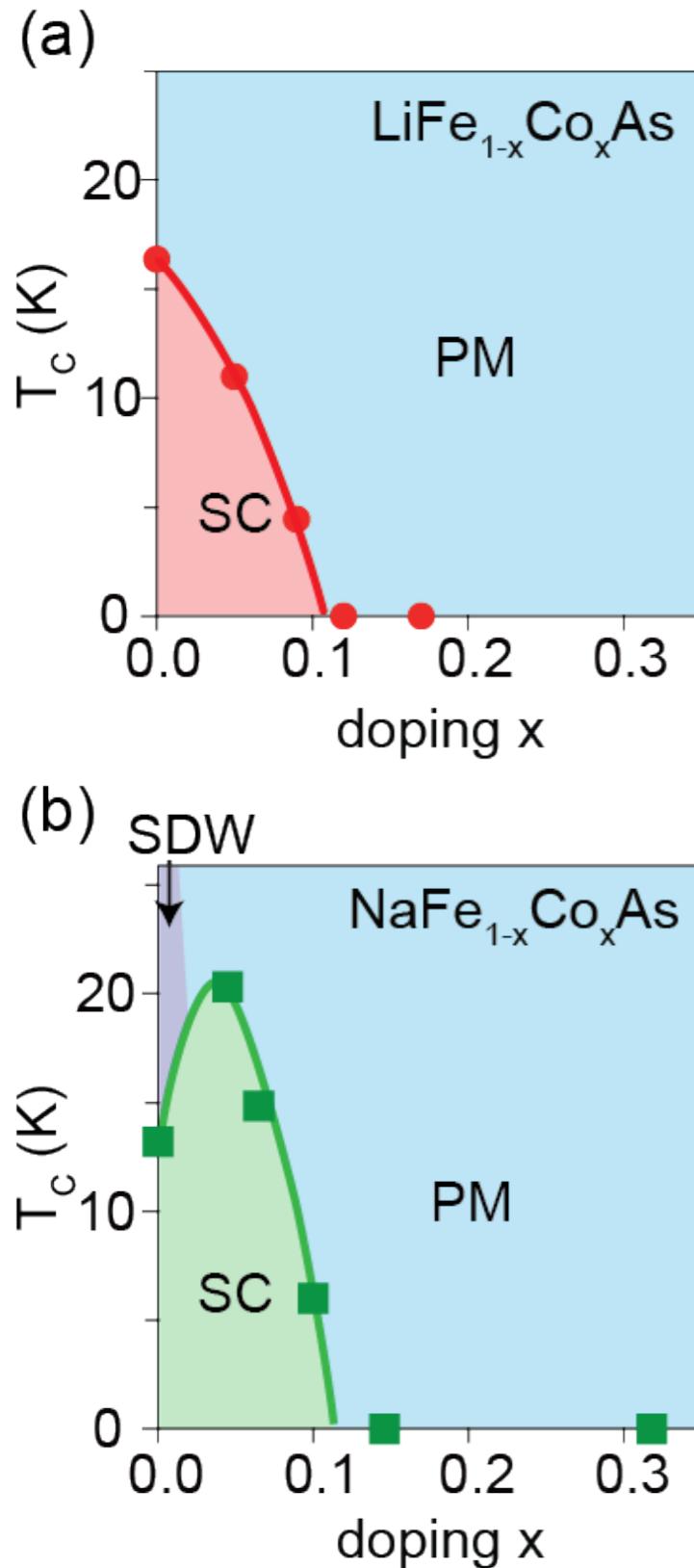
T_c=4.4K

T_c~0K

The only correct rule:

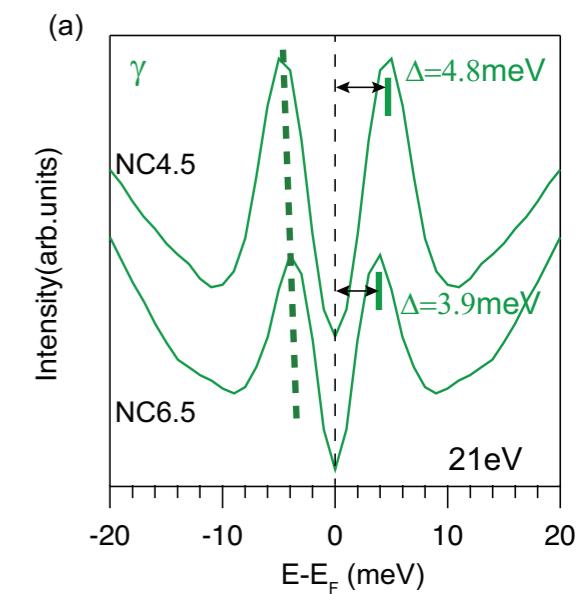
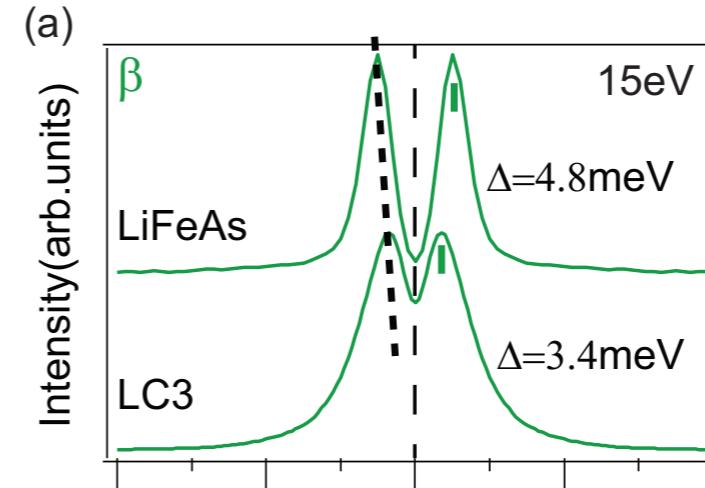
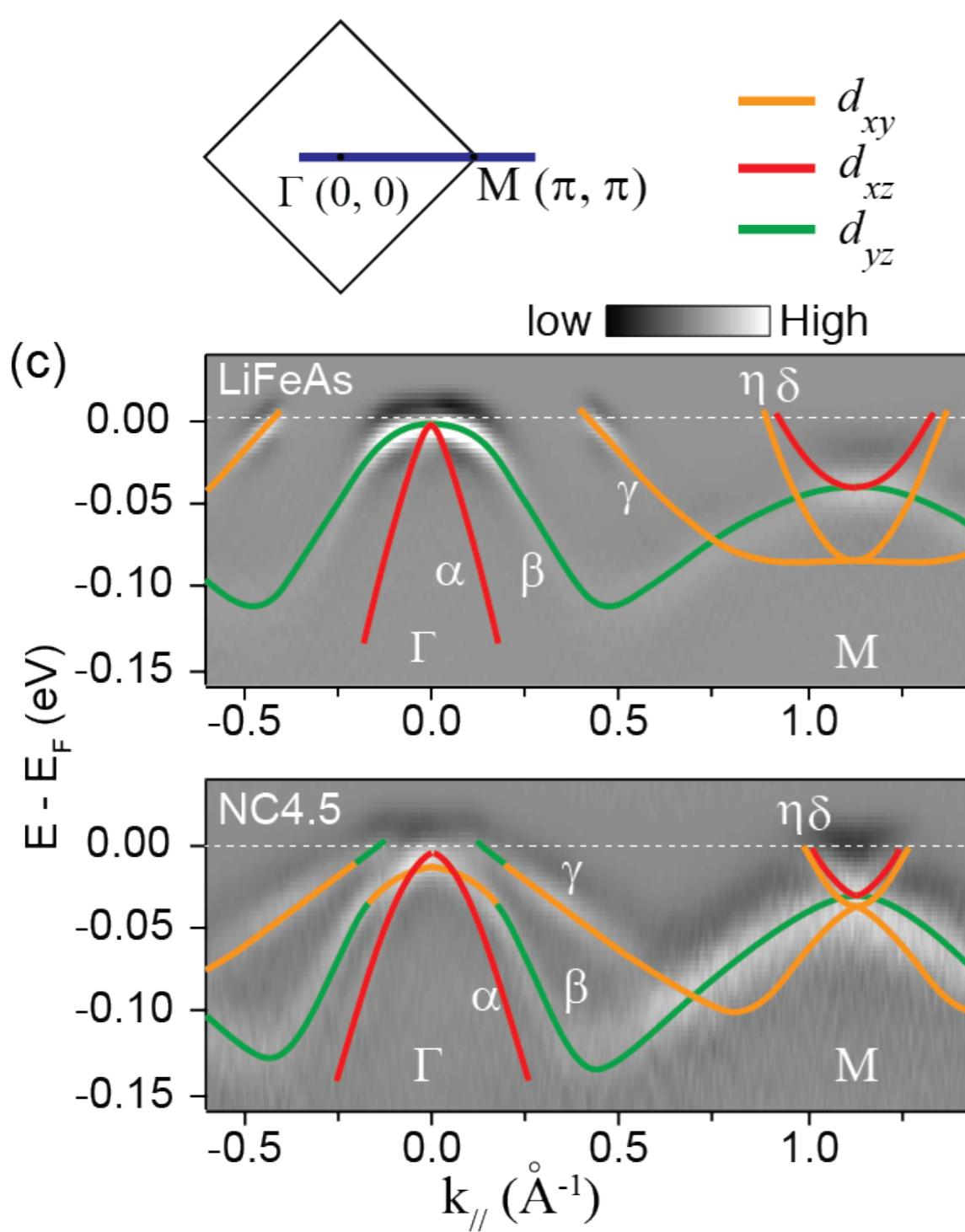
For every empirical rule regarding what determines T_c ,
there is an counter example !!

$\text{NaFe}_{1-x}\text{Co}_x\text{As}$ and $\text{LiFe}_{1-x}\text{Co}_x\text{As}$



The superconductivity is tuned from $T_c=20\text{K}$ to 0K by doping cobalt.

$\text{NaFe}_{1-x}\text{Co}_x\text{As}$ and $\text{LiFe}_{1-x}\text{Co}_x\text{As}$



1. **High sample quality and nonpolar surface**
 - clean band dispersion.
 - Sharp superconducting peaks
2. **Simple orbital characters of various bands**
 - The d_{xy} bands is very different for these two systems

Ideal systems for ARPES to study the role of orbital degree of freedom.

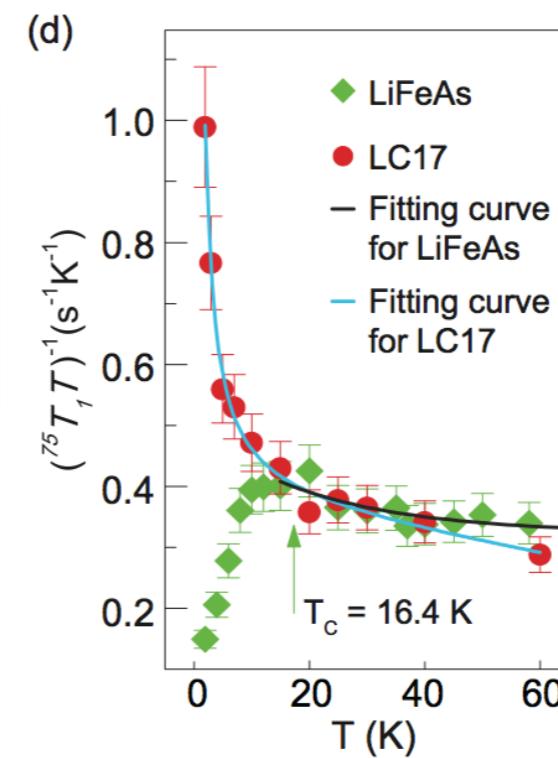
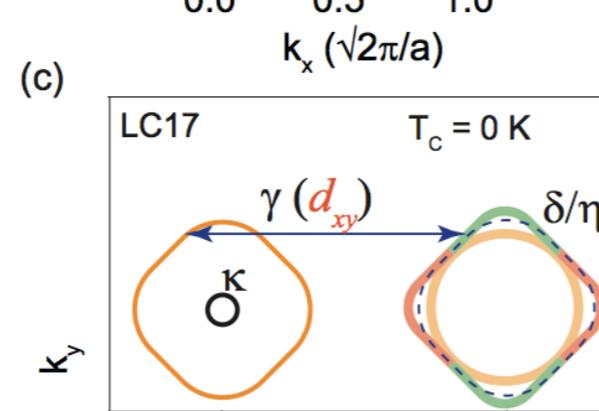
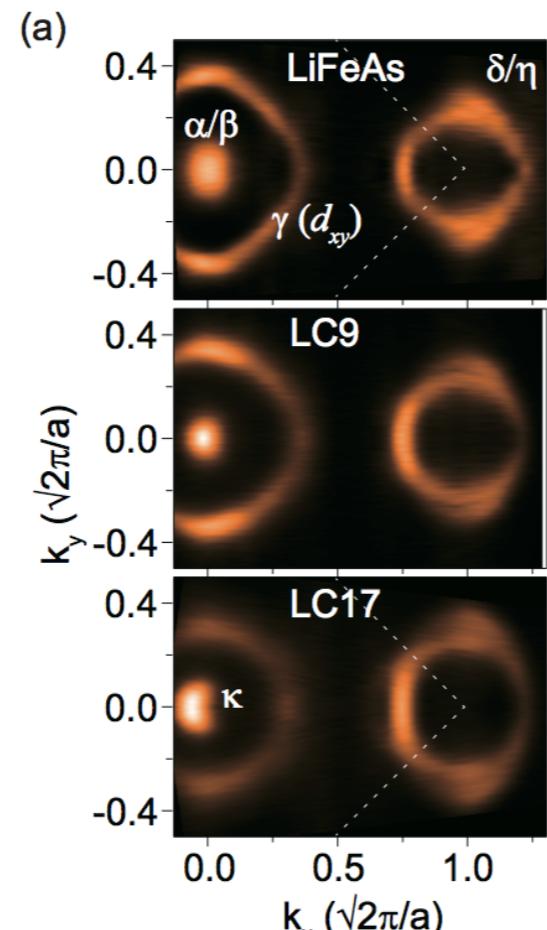
Nesting condition tuning, and orbital selectivity

Better or perfect
nesting for d_{xz}
hole pocket

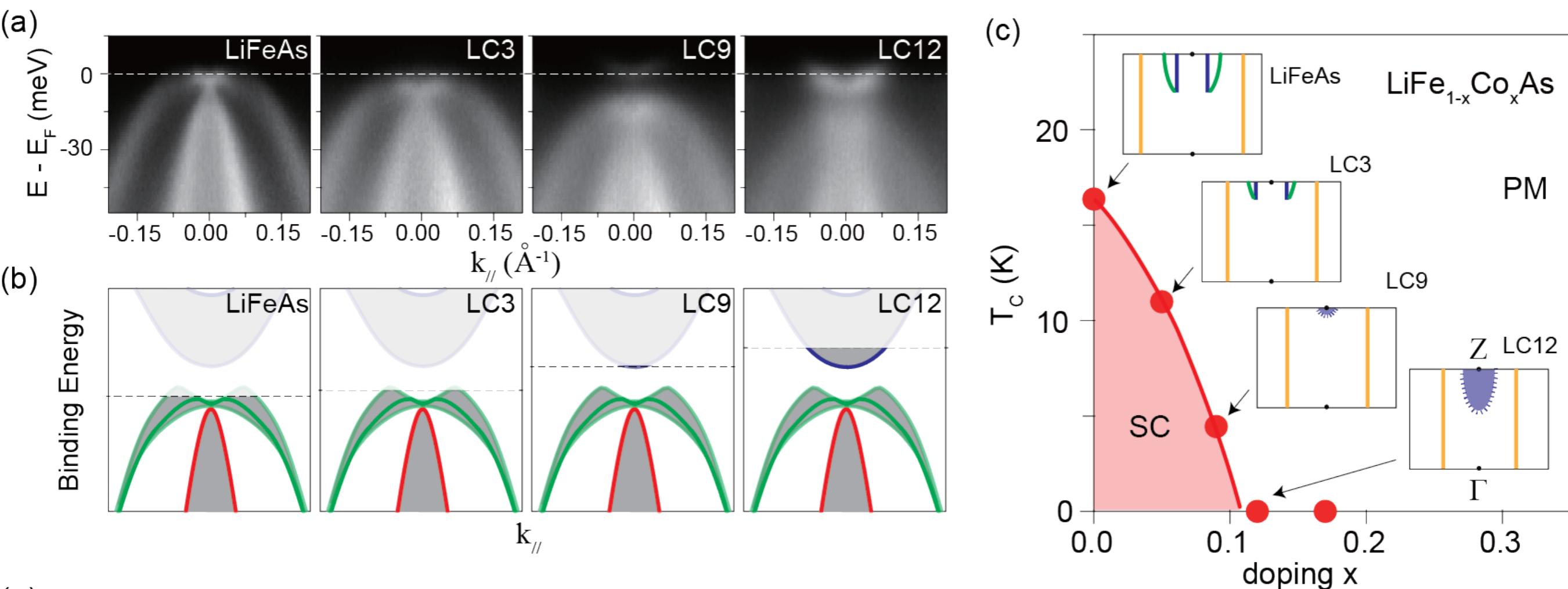


Enhance low-energy
spin fluctuations

Does not help SC
or induce SDW



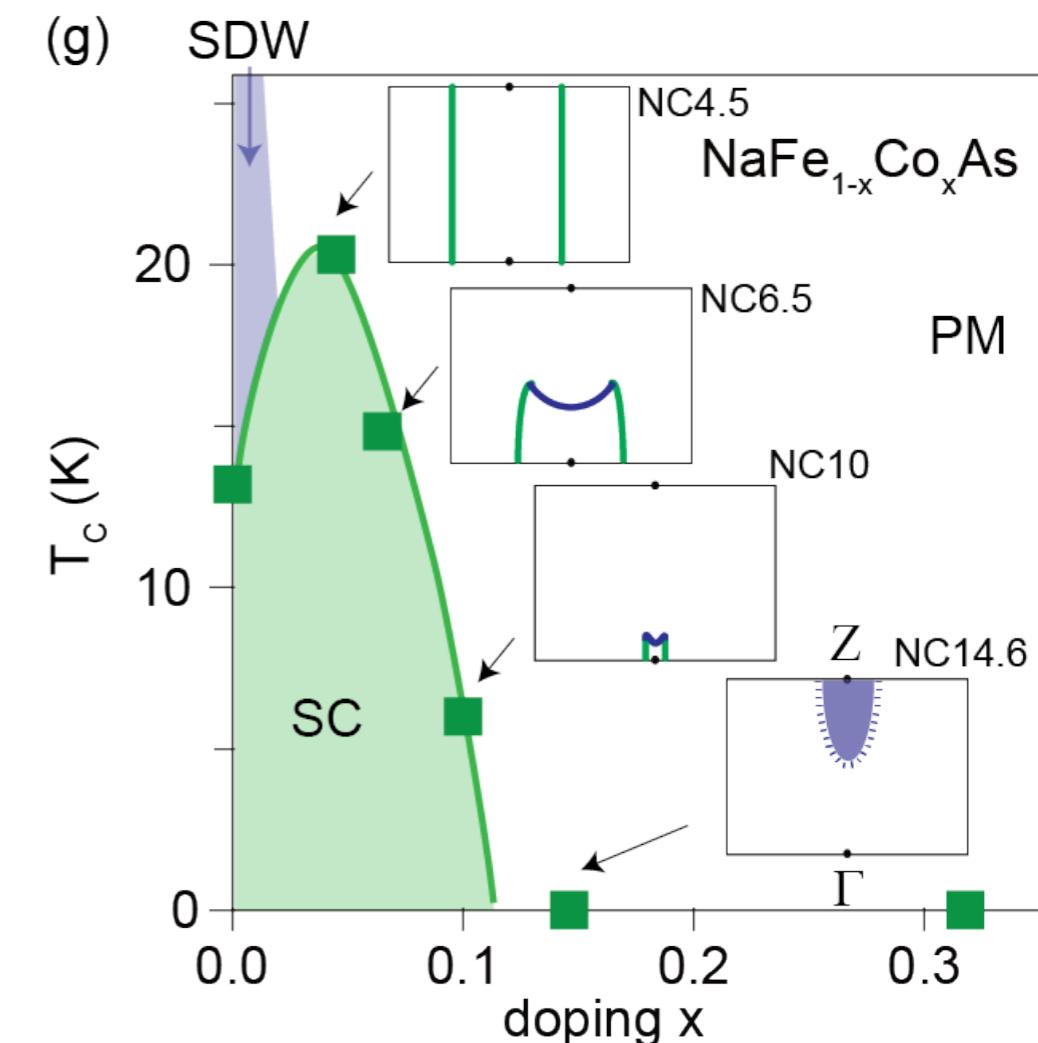
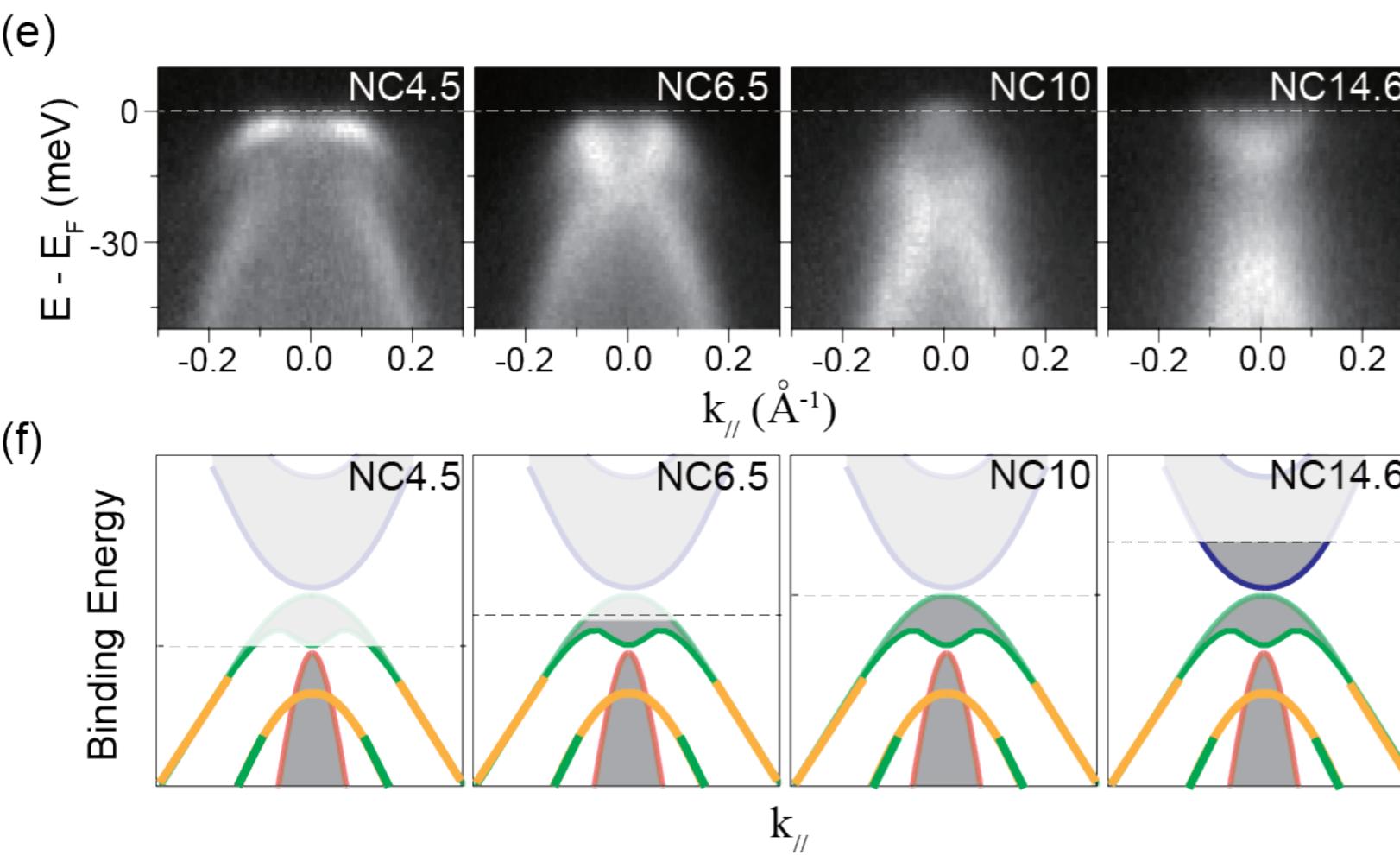
Lifshitz transition in $\text{LiFe}_{1-x}\text{Co}_x\text{As}$



The Lifshitz transition of dxz and dyz pockets

1. The dxz/dyz Fermi surface shrinks and sinks below E_F around the Z point.
2. The κ electron pocket emerges around Z in LC9 and LC12.

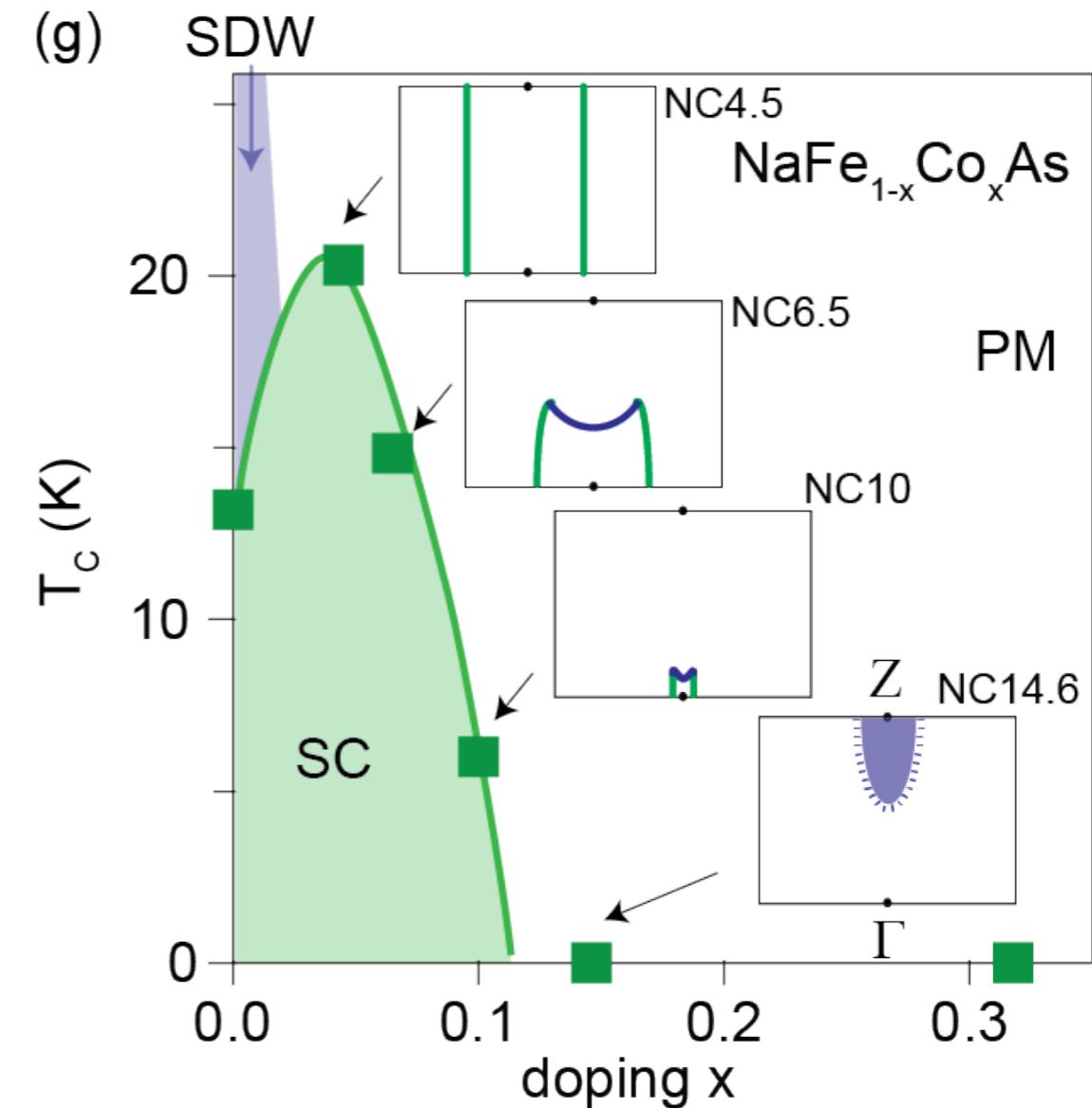
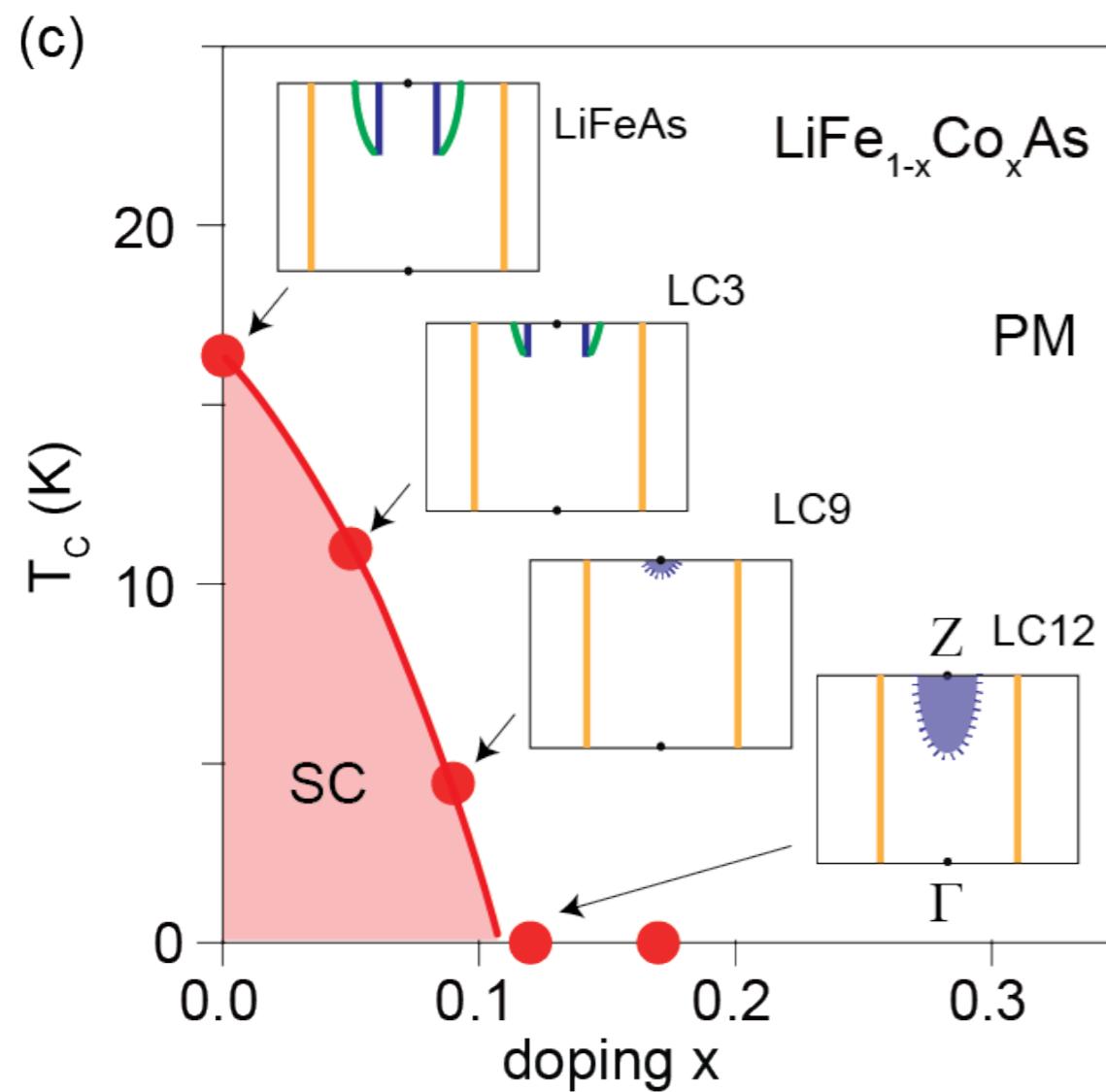
Lifshitz transition in $\text{NaFe}_{1-x}\text{Co}_x\text{As}$



The Lifshitz transition of dxz and dyz pockets

1. The dxz/dyz Fermi surface shrinks and sinks below E_F around the Γ point.
2. The κ electron pocket emerges around Z in NC14.6.

The critical role of central dxz/dyz hole Fermi surfaces



Shortly after the Lifshitz transition of dxz/dyz Fermi surface. (The topology does not matter, differs a lot.)

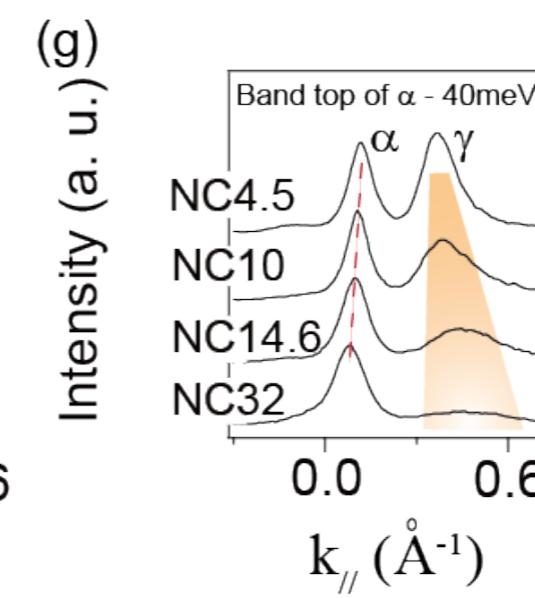
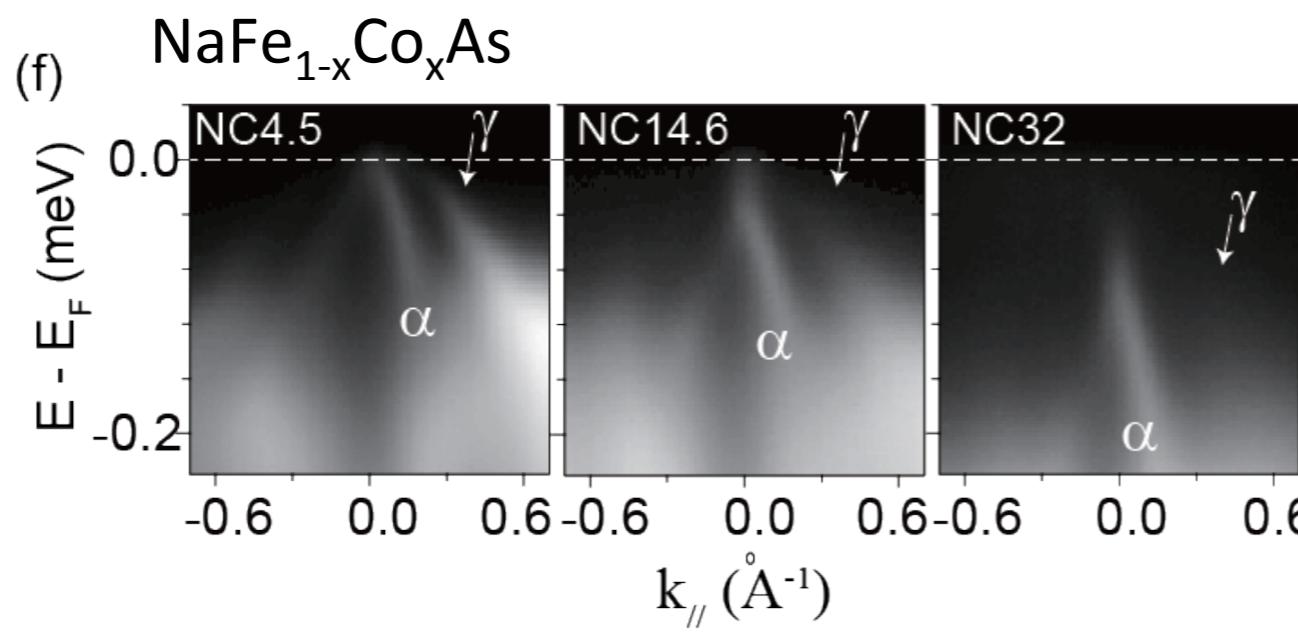
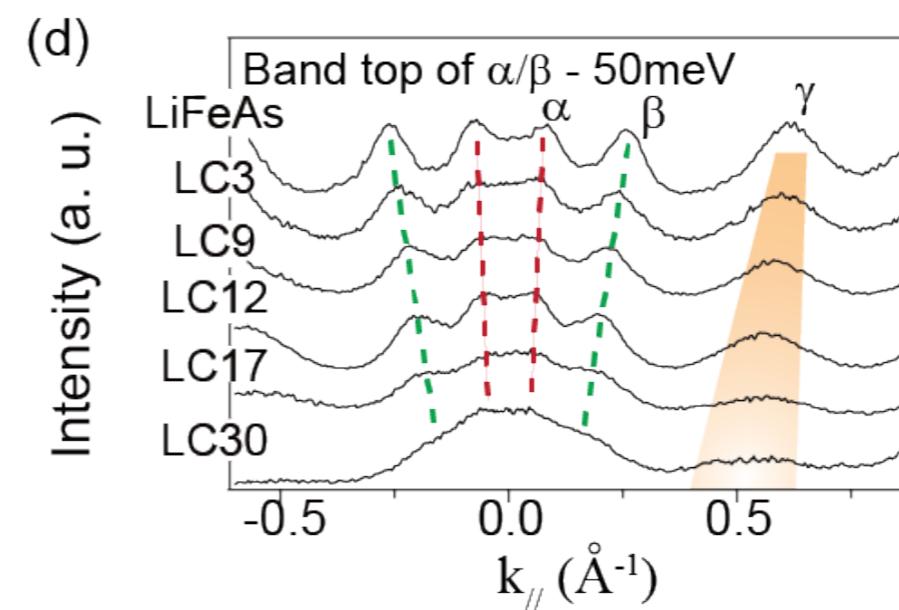
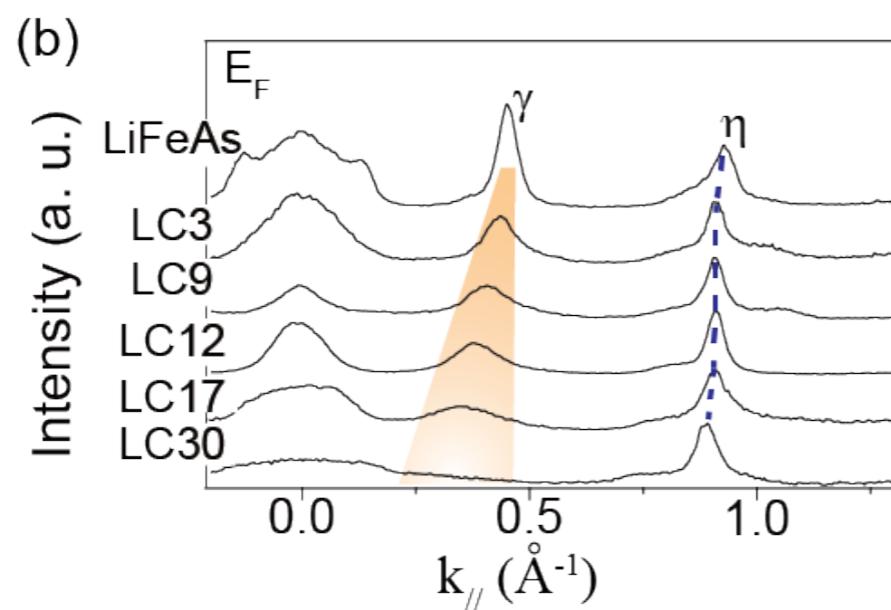
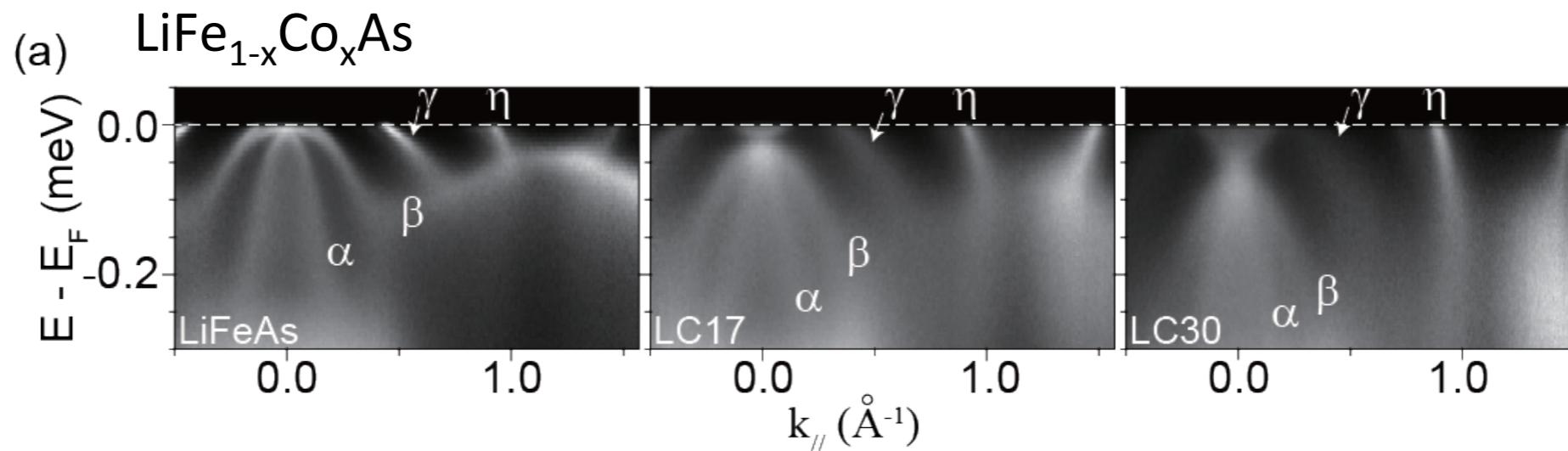
The SC to non-SC transition.

The presence of dxz/dyz hole Fermi surfaces appears critical for SC. After dxz/dyz hole FS disappear, there is some residual superconductivity contributed by all other FS.

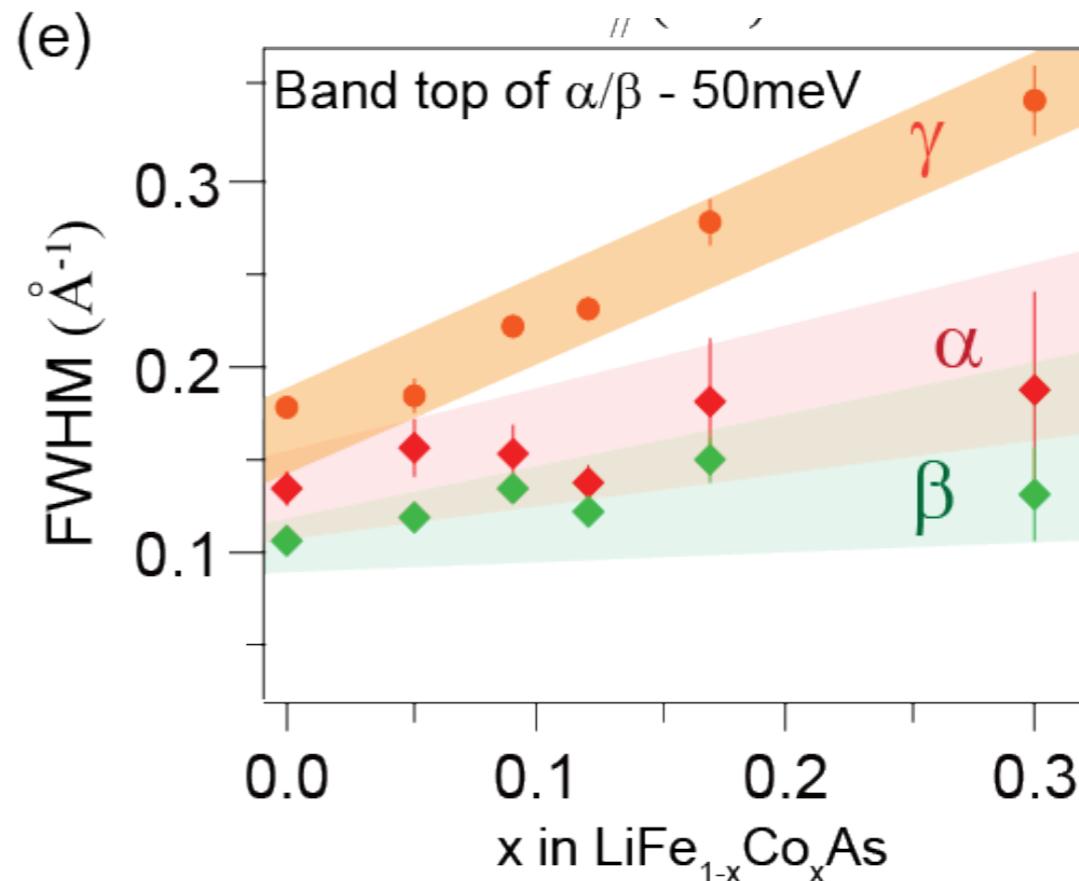
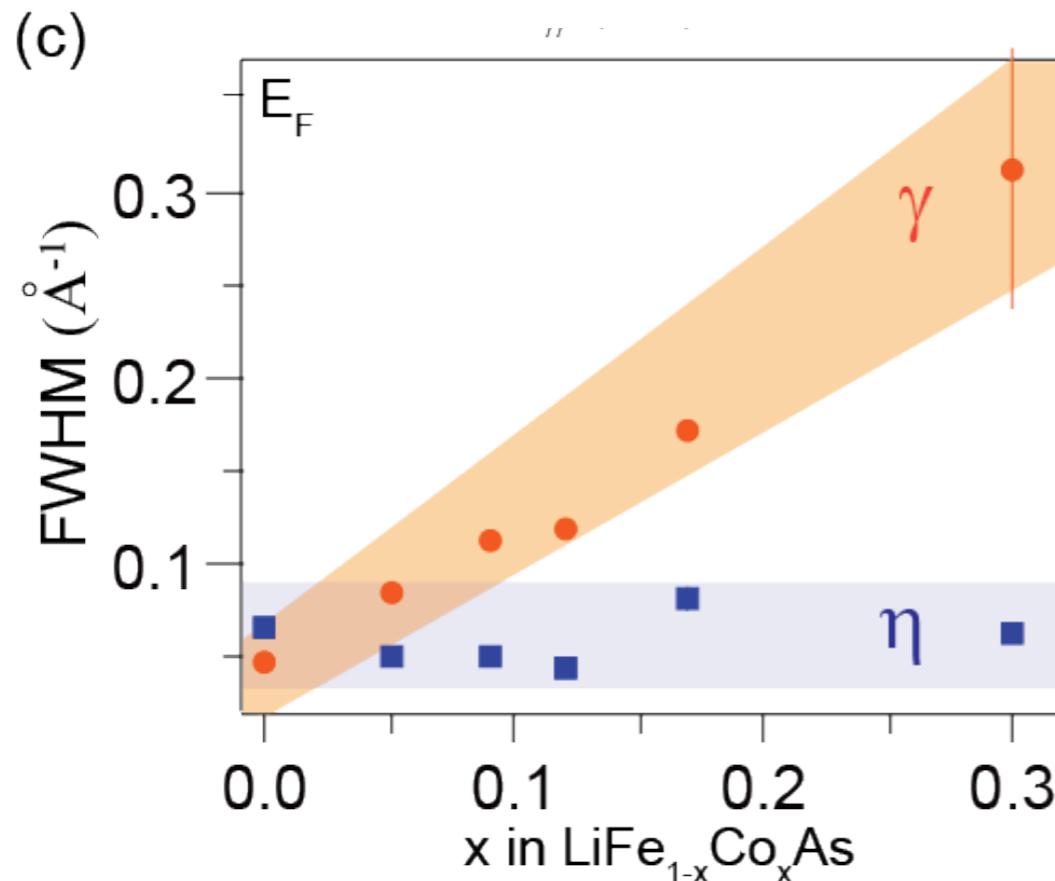
**dxz/dyz orbital selective correlations between
nesting/Lifshitz transition and the
superconductivity in AFe_{1-x}Co_xAs (A=Li, Na)**

What happens to the dxy hole band?

Orbital selective impurity scattering



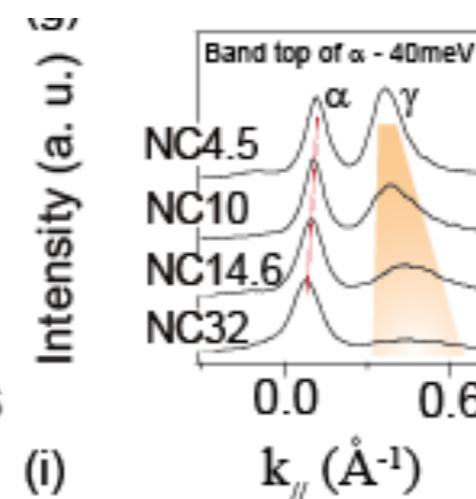
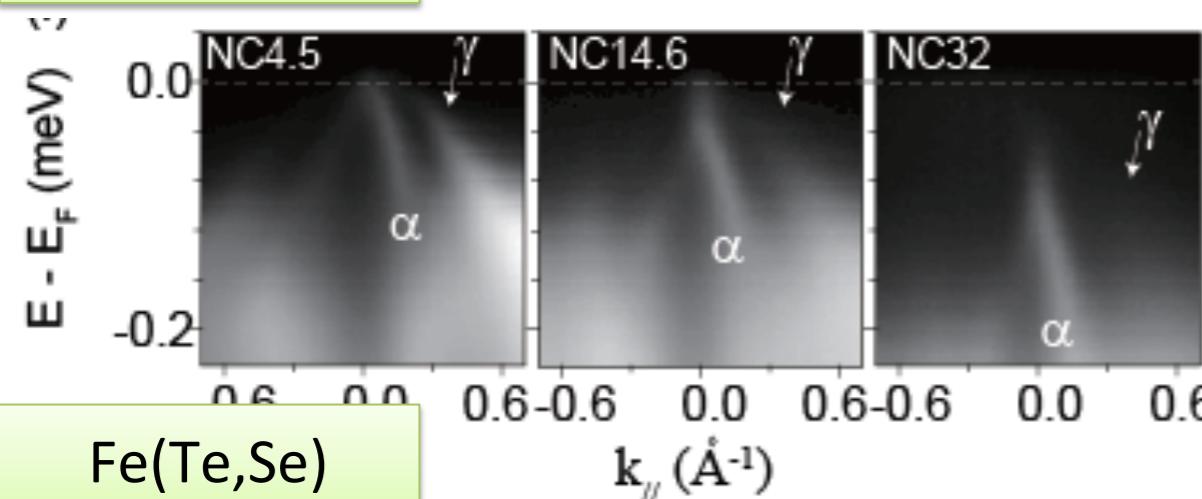
Orbital selective impurity scattering



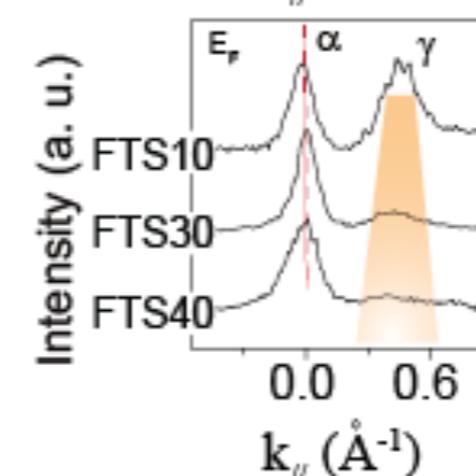
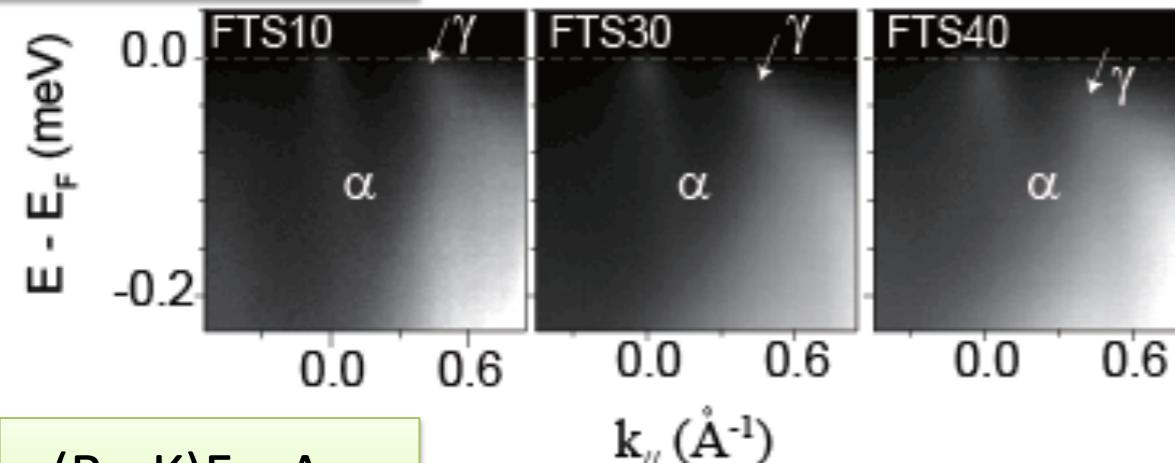
- The dxz/dyz bands(α and β) are rather insensitive to impurity scattering.
- The dxy band (γ) is strongly suppressed and broadened.
- Explain the robust superconductivity against heavy doping in iron-based superconductors.
- Explain STM data of “weak” Co-impurity in NaFeAs

The defect location is critical for impurity scattering

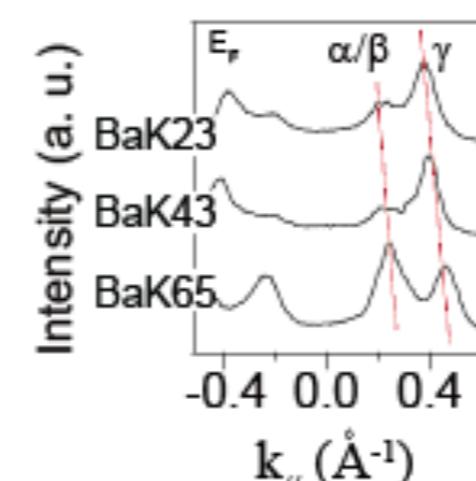
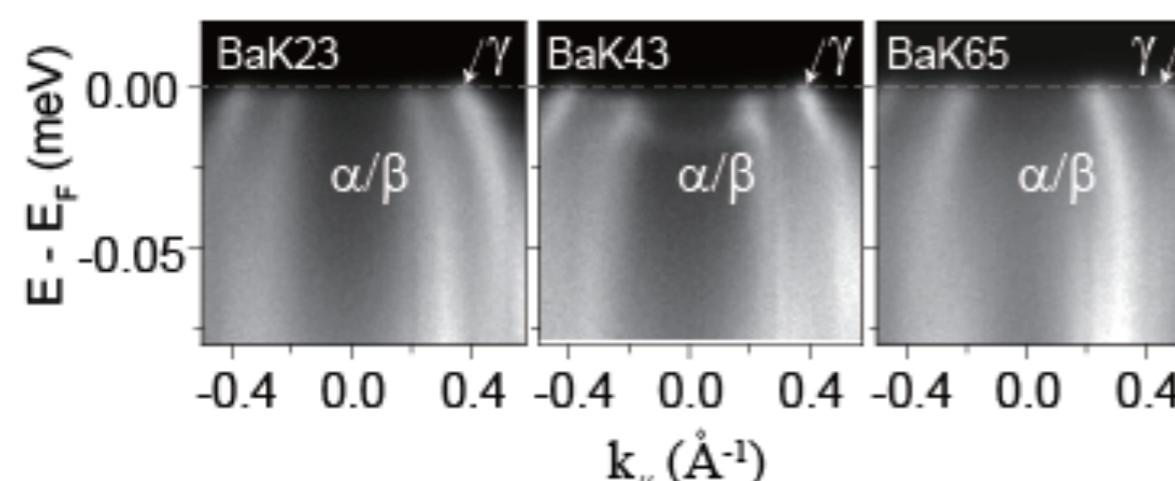
Na(Fe,Co)As



Fe(Te,Se)



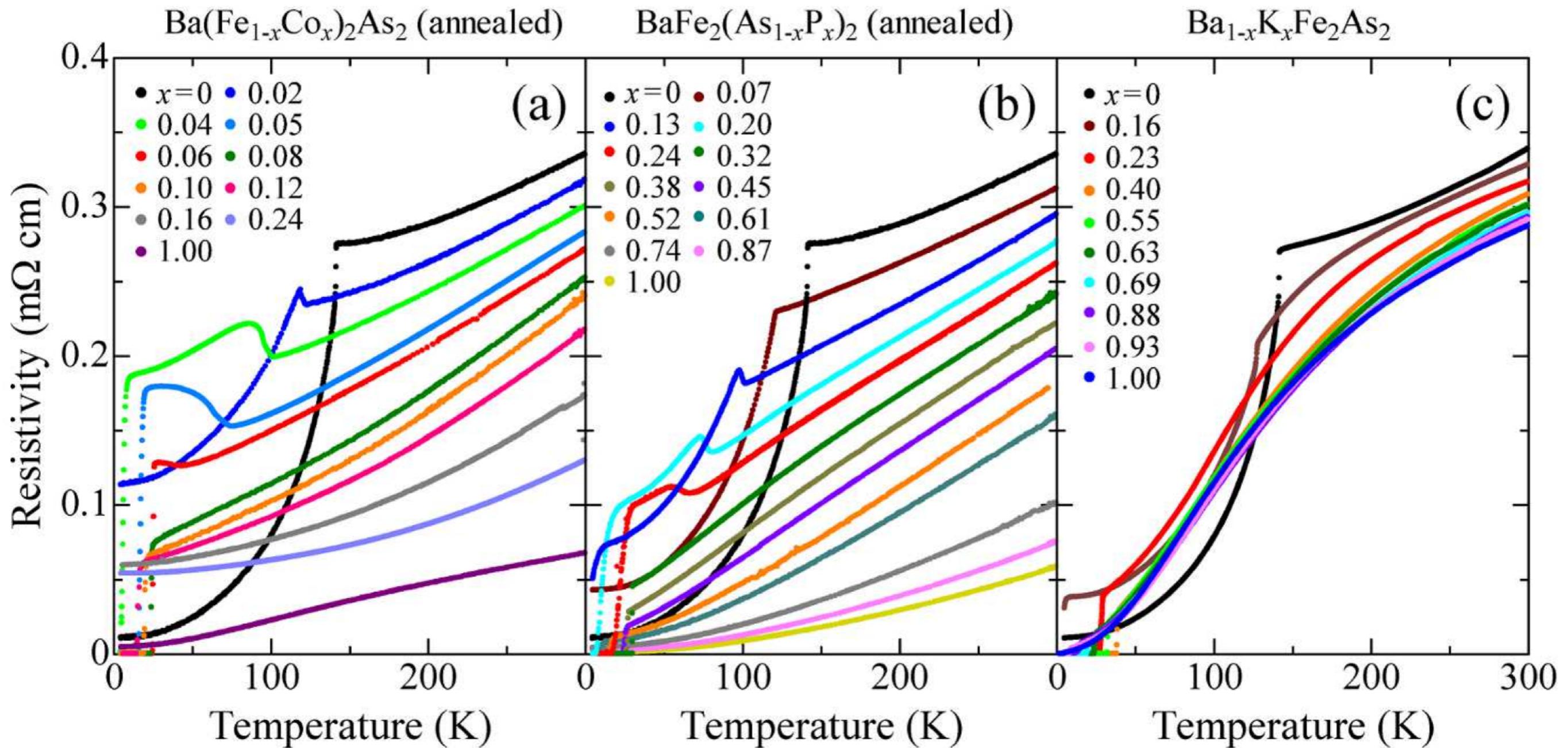
(Ba,K)Fe₂As₂



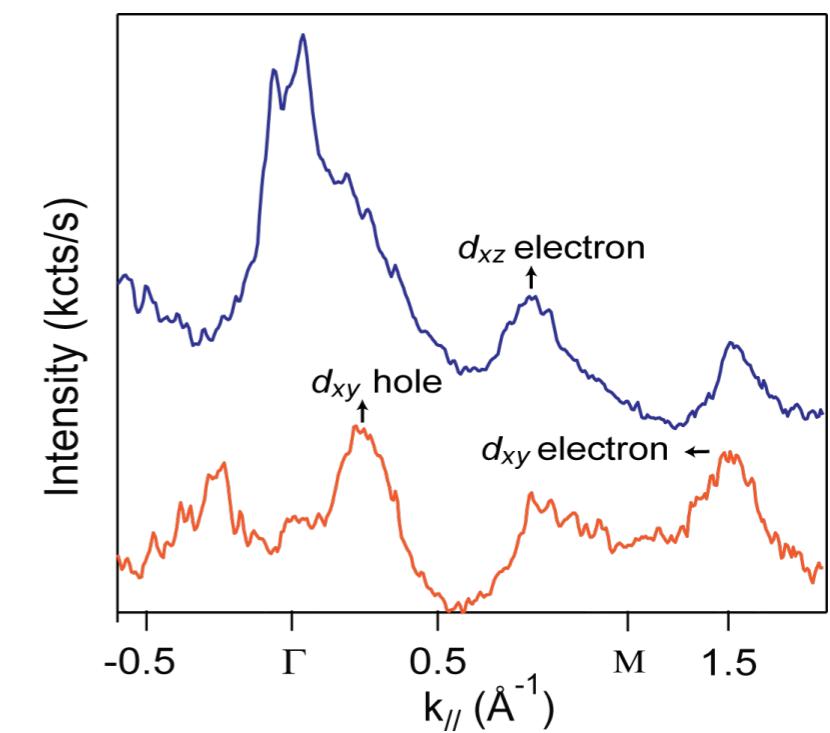
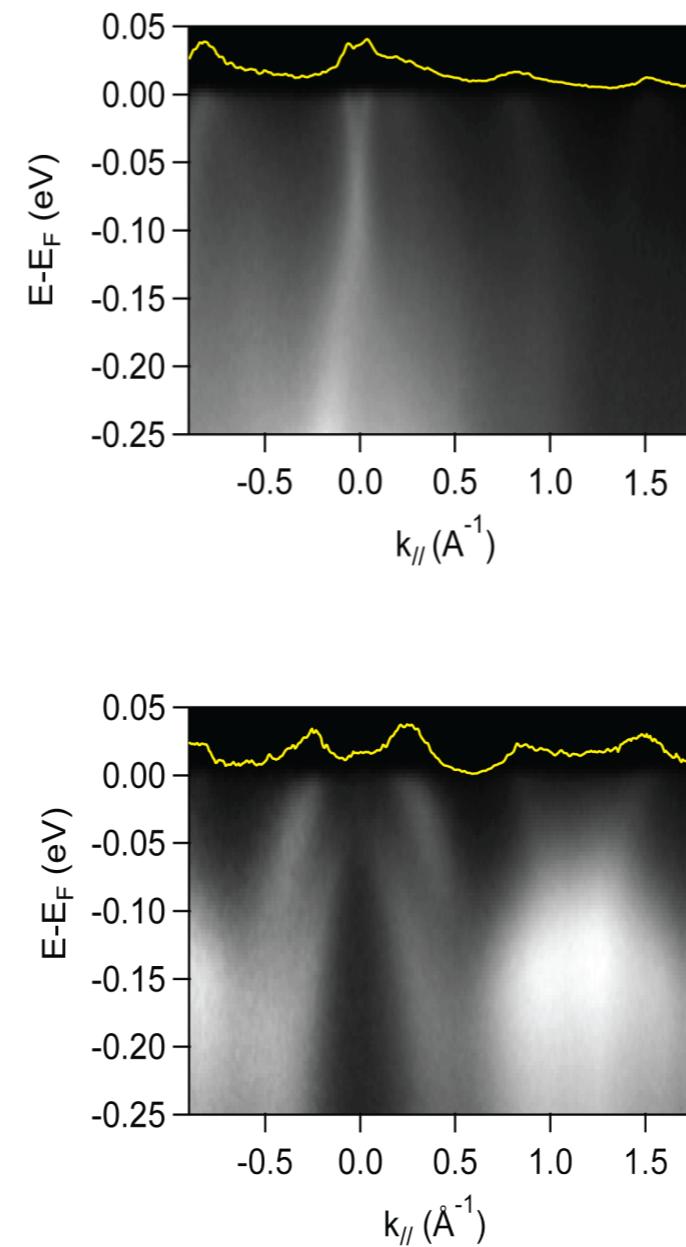
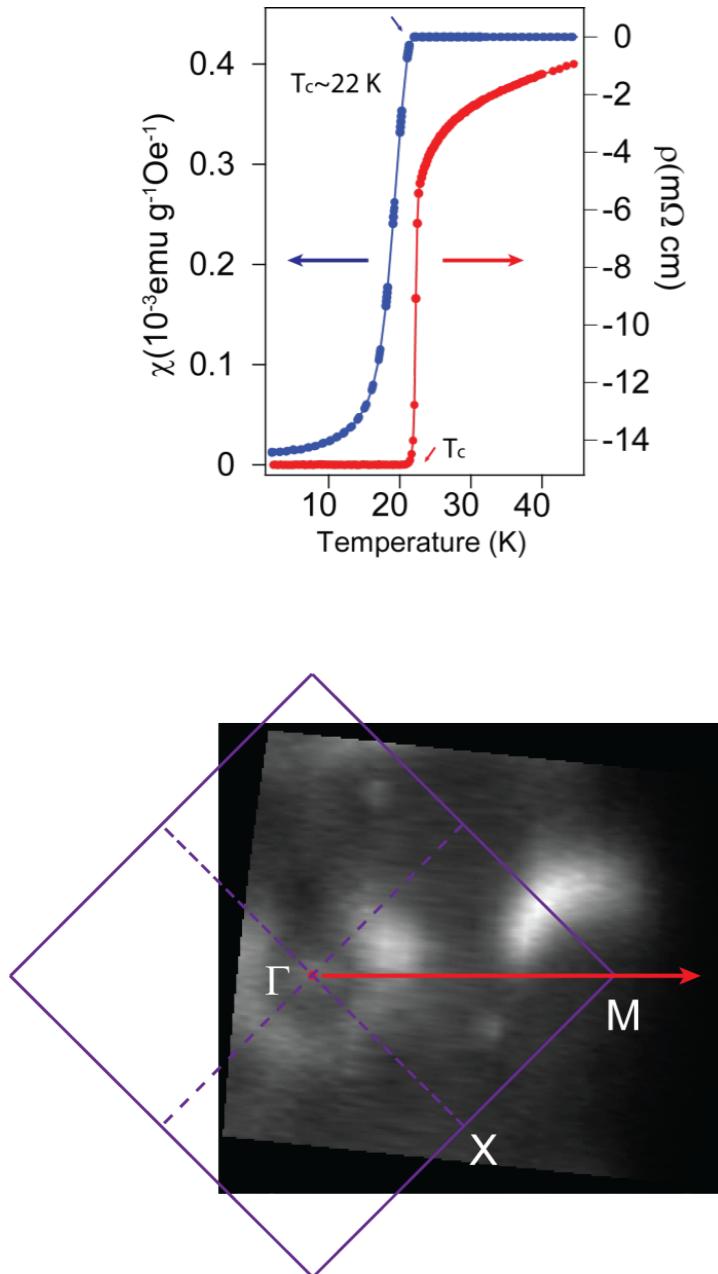
1. Doping in the FeAs(Se) plane:
The hole dxy band (γ) is strongly suppressed and broadened !?

2. Doping out of the FeAs plane:
All the bands are relatively unchanged with dopants.

Impurity effects on resistivity



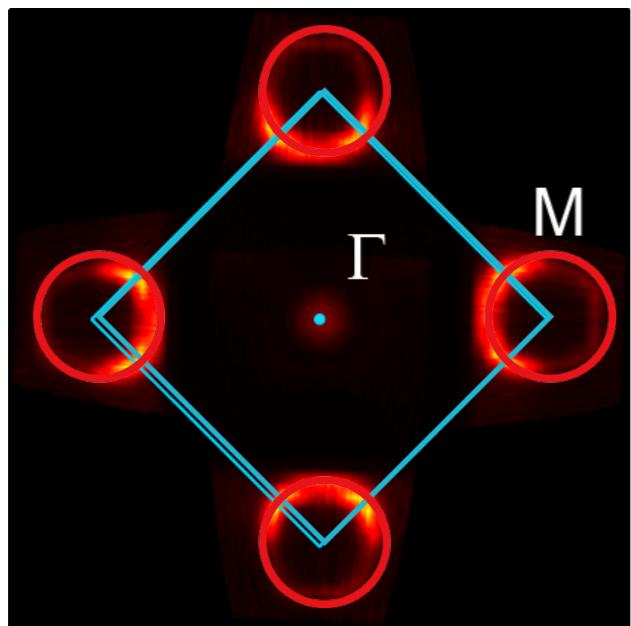
When d_{xy} hole band is not strongly scattered: 22K superconductivity in Ca₁₀(Pt₄As₈)(Fe_{2-x}Pt_xAs₂)₅



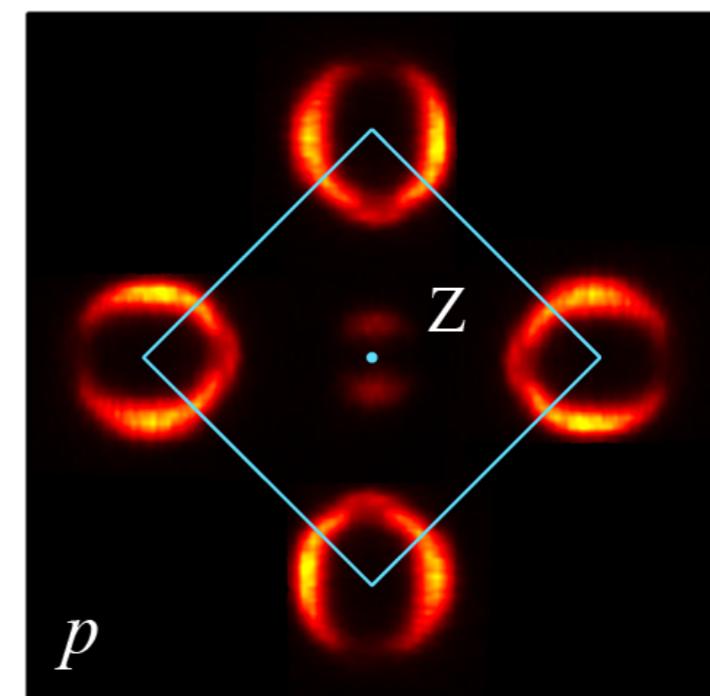
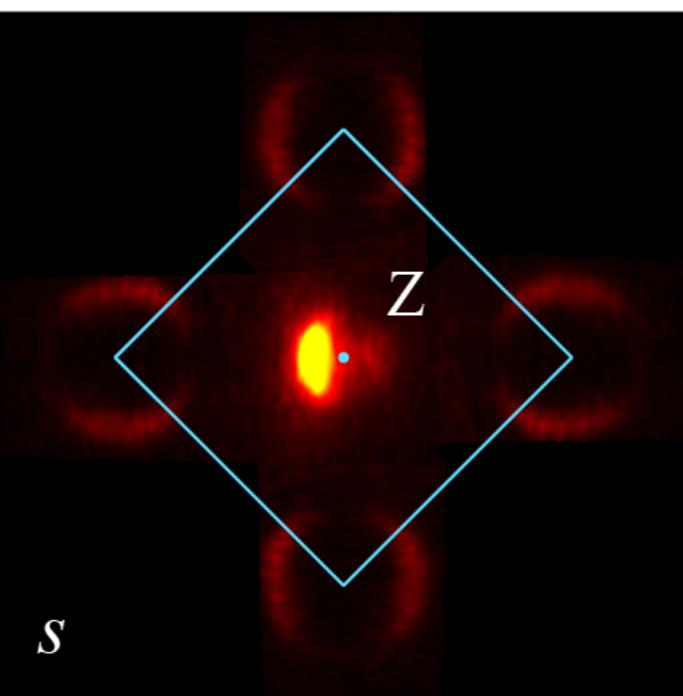
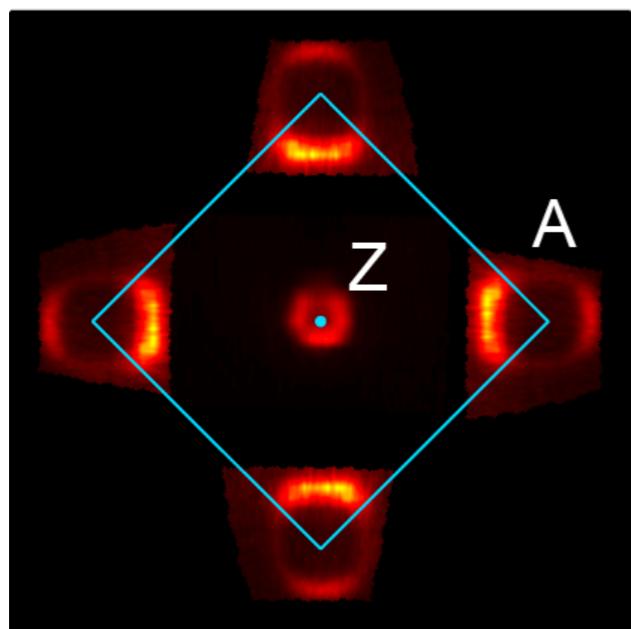
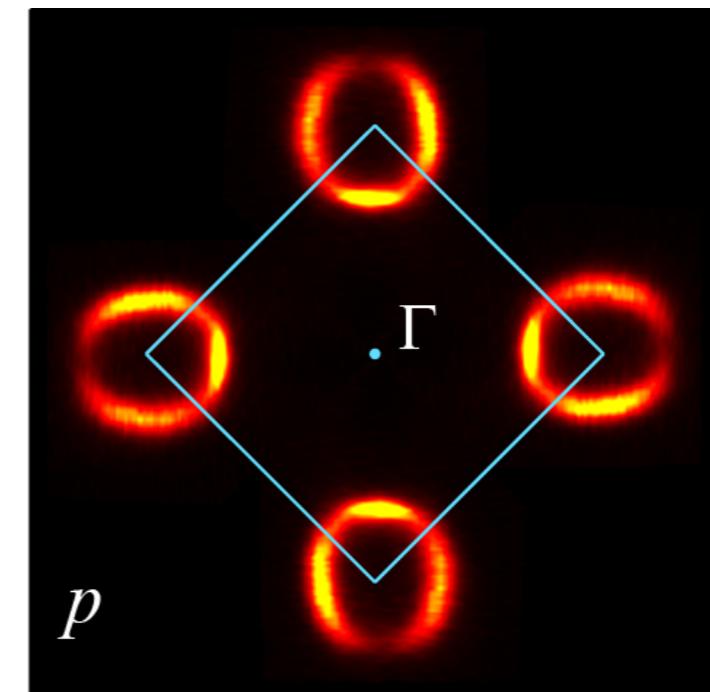
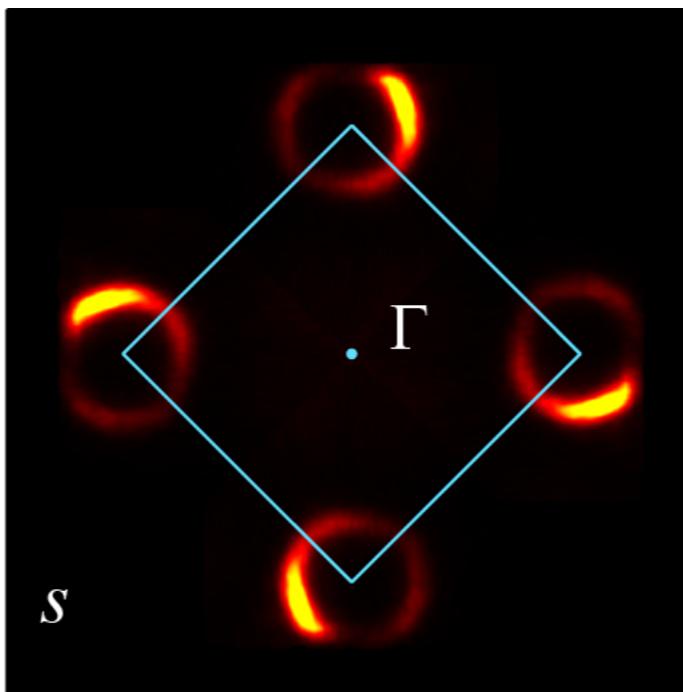
Comparable d_{xy} scattering rate with others

Electron-only Fermi surface of $\text{NaFe}_{0.7}\text{Co}_{0.3}\text{As}$

$\text{K}_x\text{Fe}_{2-y}\text{Se}_2$ $T_c=31\text{K}$

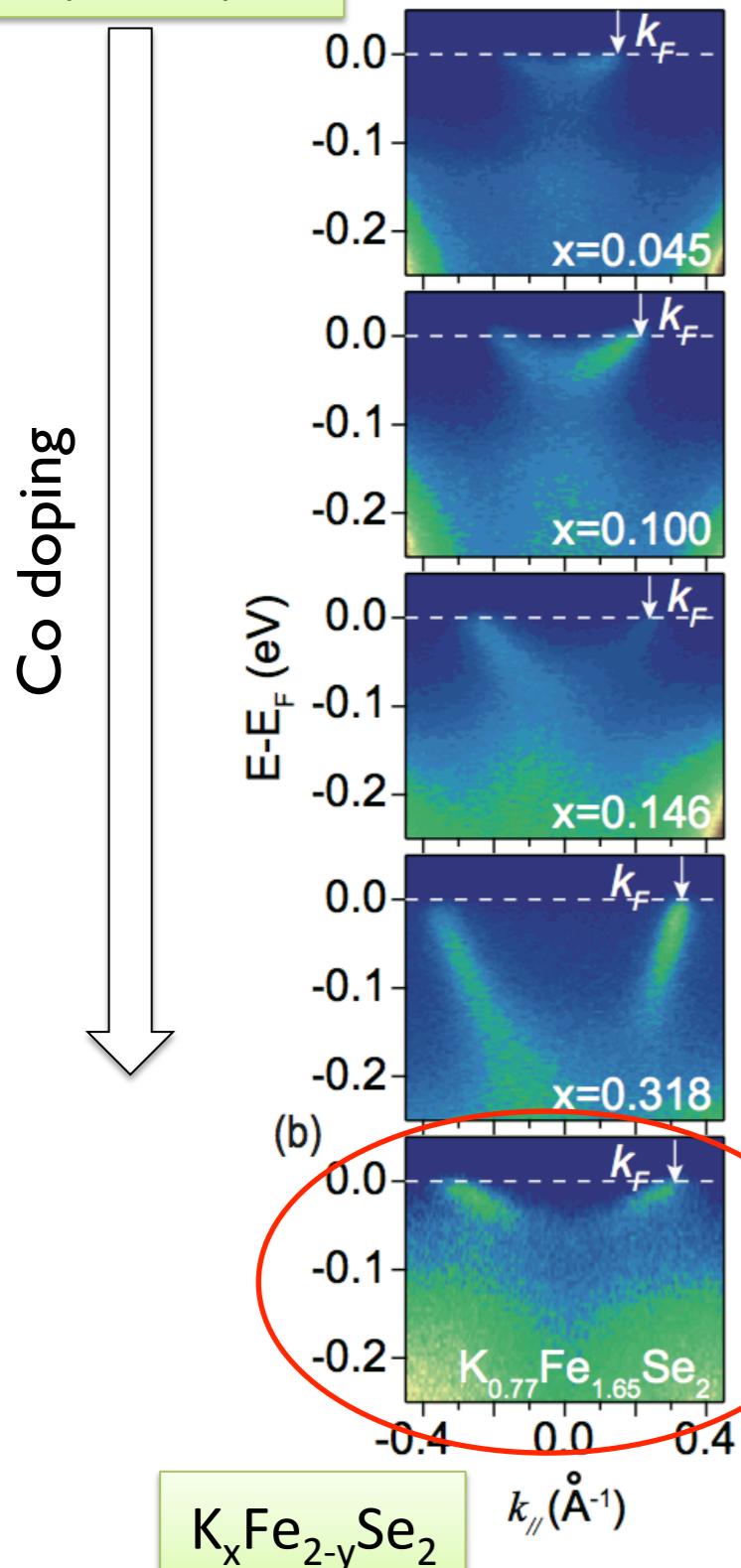


$\text{NaFe}_{0.7}\text{Co}_{0.3}\text{As}$ $T_c=0\text{K}$

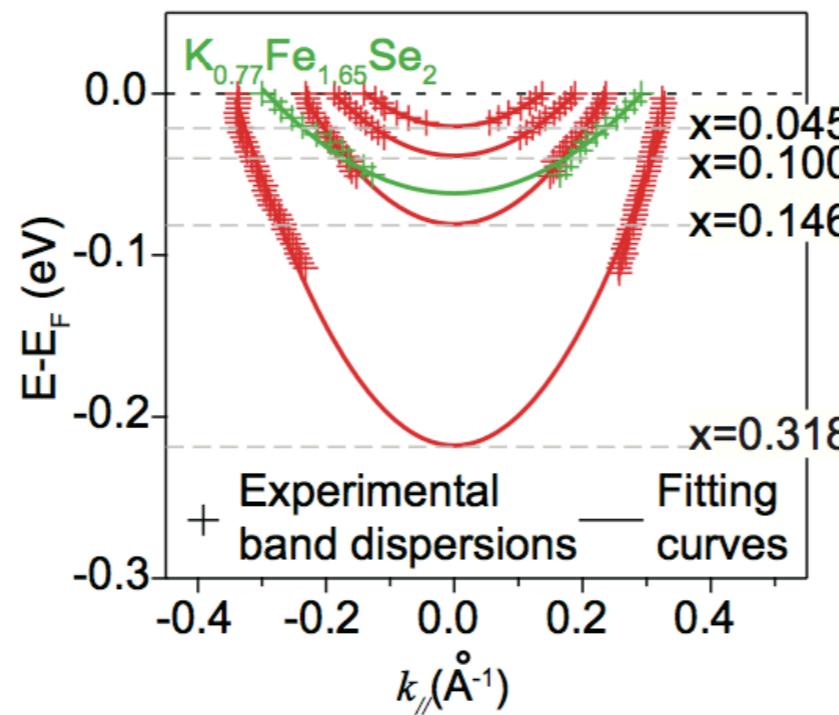


Sizable correlation matters

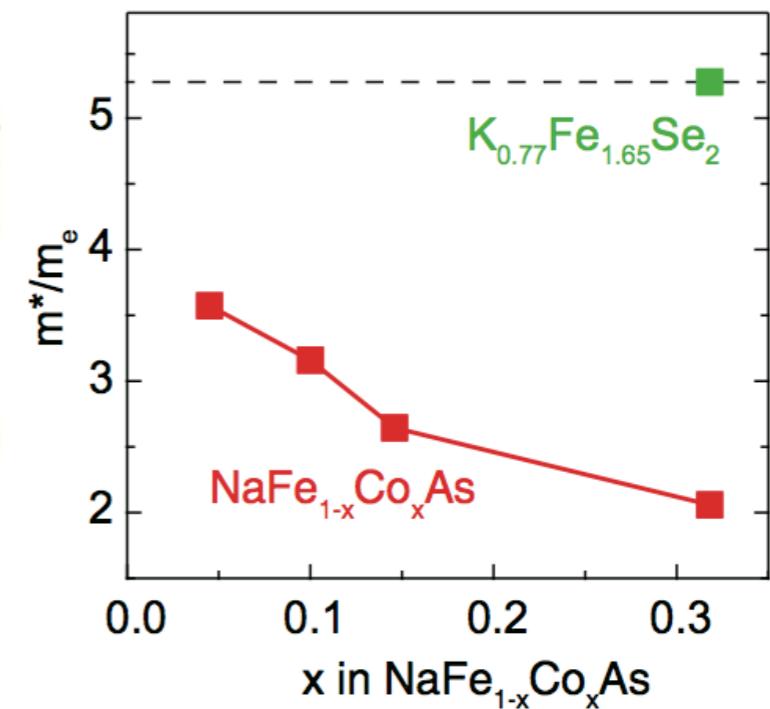
Na(Fe,Co)As



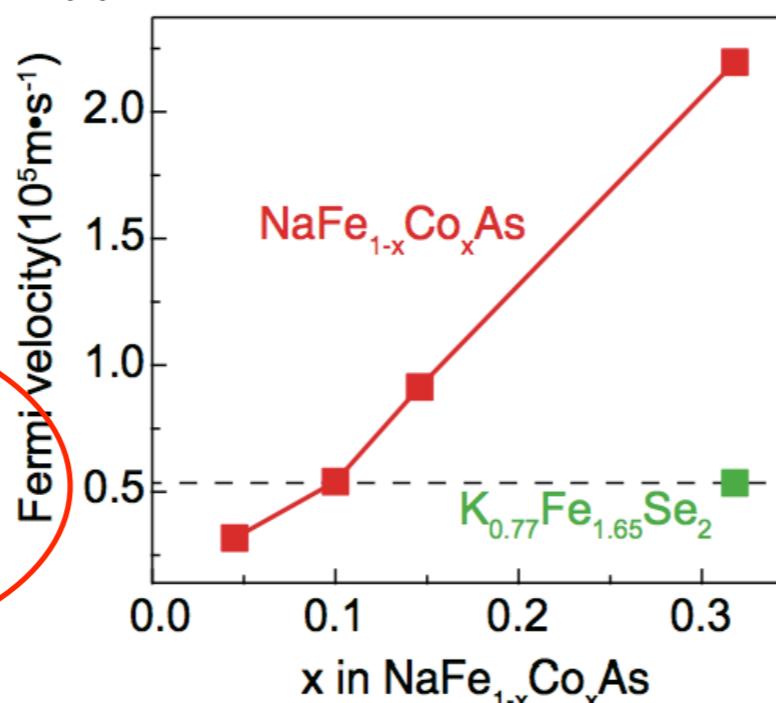
(c)



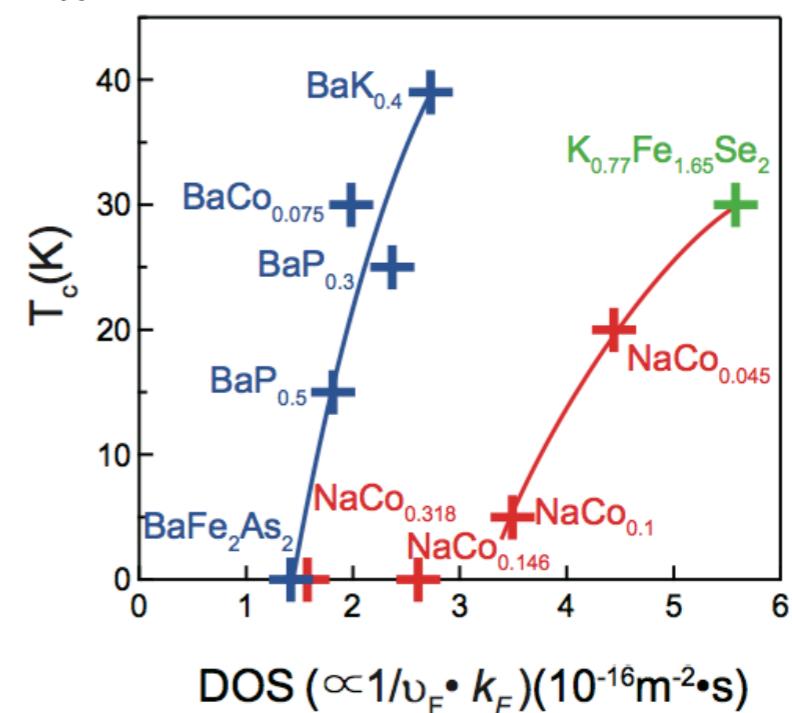
(d)



(e)

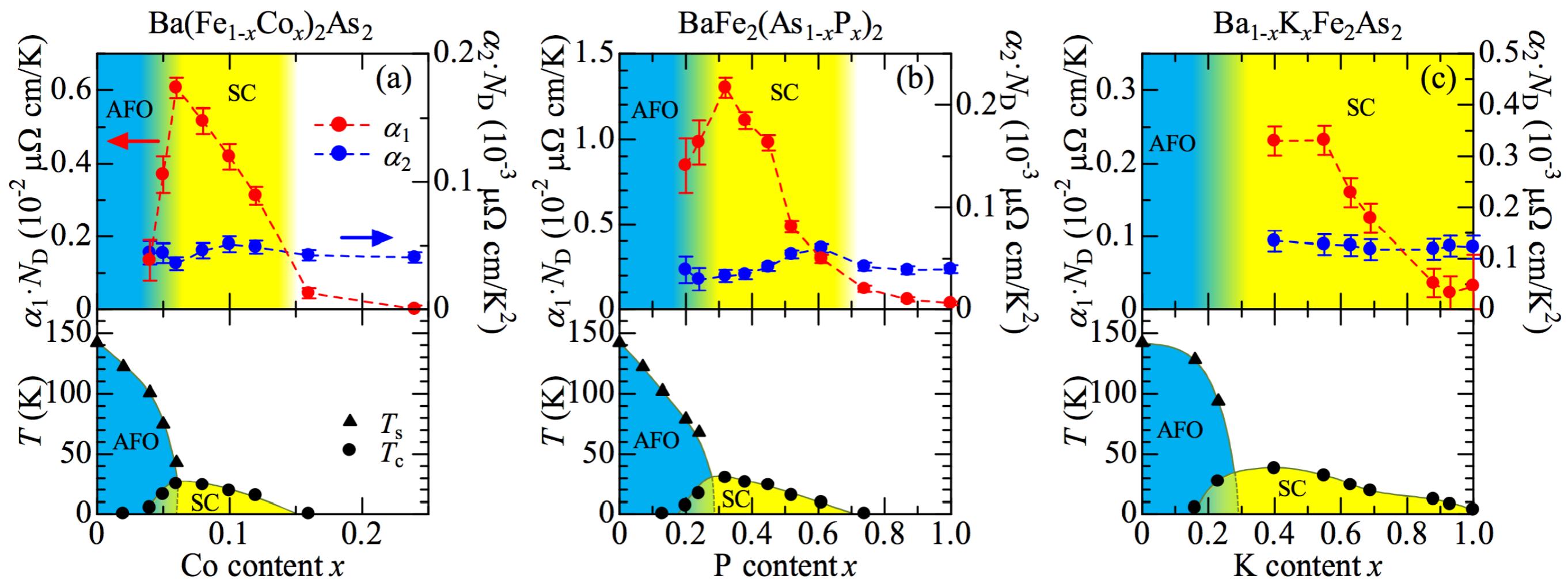


(f)



Correlations matter

$$1/\rho(T) = 1/(\rho_0 + \alpha_1 T + \alpha_2 T^2) + \sigma_{\text{in}}$$



What governs T_c for Type-I Fe-HTS's

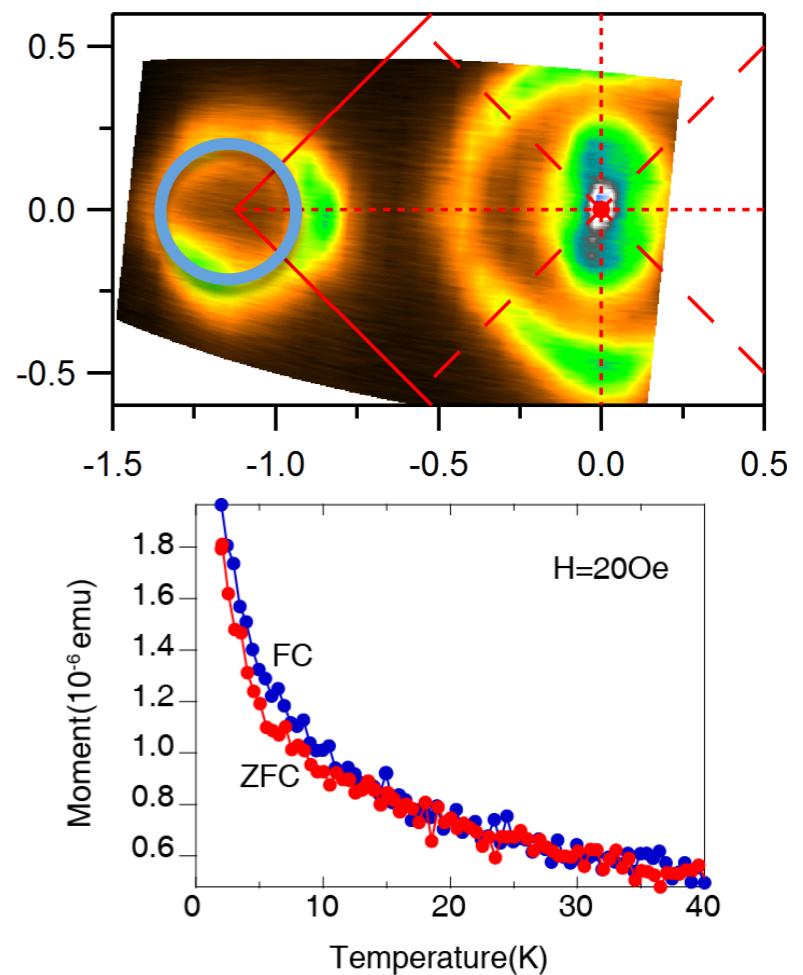
1.

Fermiology

- Good nesting helps, when other conditions are similar. For example, nesting does not work when there is strong impurities, such as strong magnetic impurity.
- T_c could be enhanced by the perfect FS nesting, e.g. between dxz/dyz-originated FSs
- The dxy hole pocket can sustain SC, just more vulnerable to impurities
- Superconductivity is suppressed when the central dxz/dyz hole pockets disappear with electron doping, but Lifshitz transition is just an accident due to the strong scattering of dxy hole FS.

LiFe_{0.9}Cr_{0.1}As No SC

Hole doping
Nesting between electron and inner dxz/dyz hole pocket



What governs T_c for Type-I Fe-HTS's

2.

Impurity effects

- Dopings are extremely heavy when compared with cuprates, and impurity effects are very important in Fe-HTS.
- Location of defects matter a lot, which directly affects phase diagram, superconductivity
- The Leading role of dxz/dyz is because they are rather insensitive to impurity scattering in most cases.
- $dxz/dyz/dxy$ are all important

What governs T_c for Type-I Fe-HTS's

3.

Correlations (spin fluctuations)

- Sizable correlations are important, which are characterized by
 - ✓ proximity to the magnetic phase
 - ✓ Van Hove singularity
 - ✓ band renormalization, Fermi velocity
 - ✓ Linear term in resistivity vs. T
- NMR shows that the low-energy spin fluctuations are enhanced by nesting, but not that relevant to SC.
- INS suggests high energy ($\sim J$ scale) fluctuations may matter more (cf. Pengcheng, Elbio, Jiangping's recent review)

1.

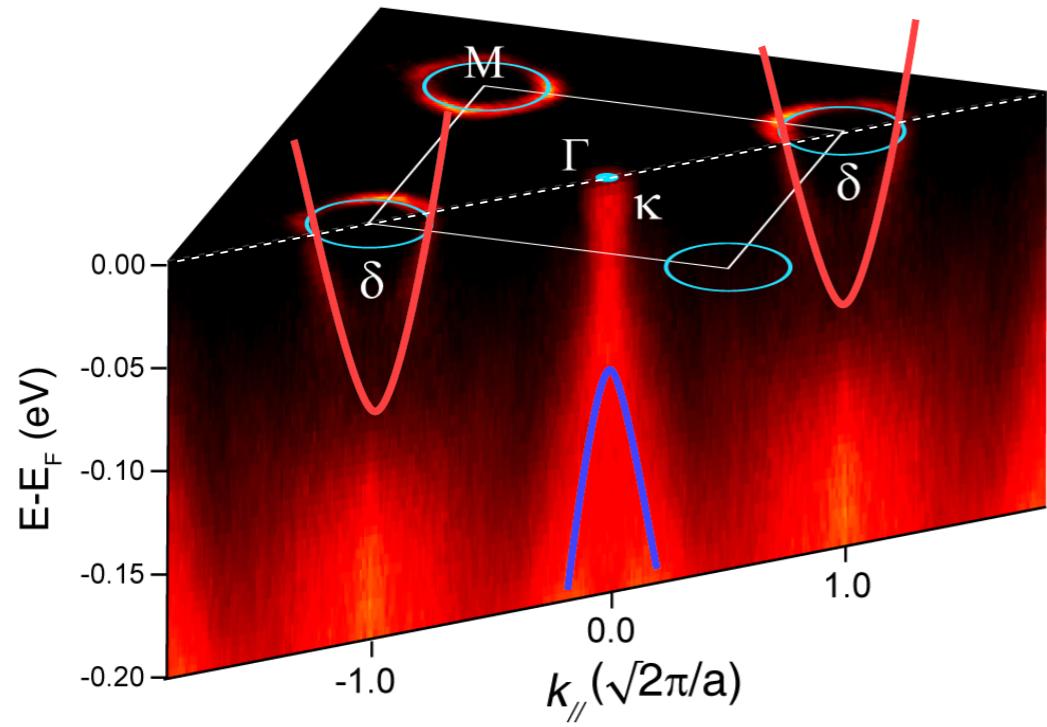
Systems with both electron and hole pockets

2.

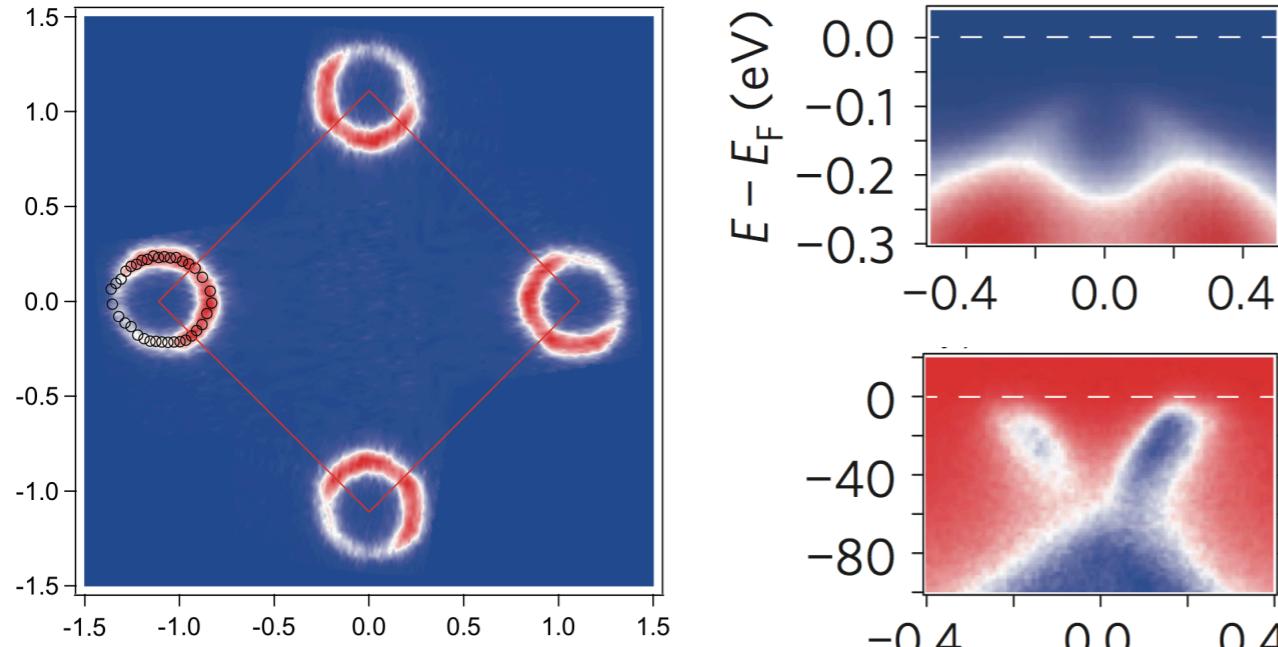
Systems with only electron pockets

Type-II Fe-HTS's

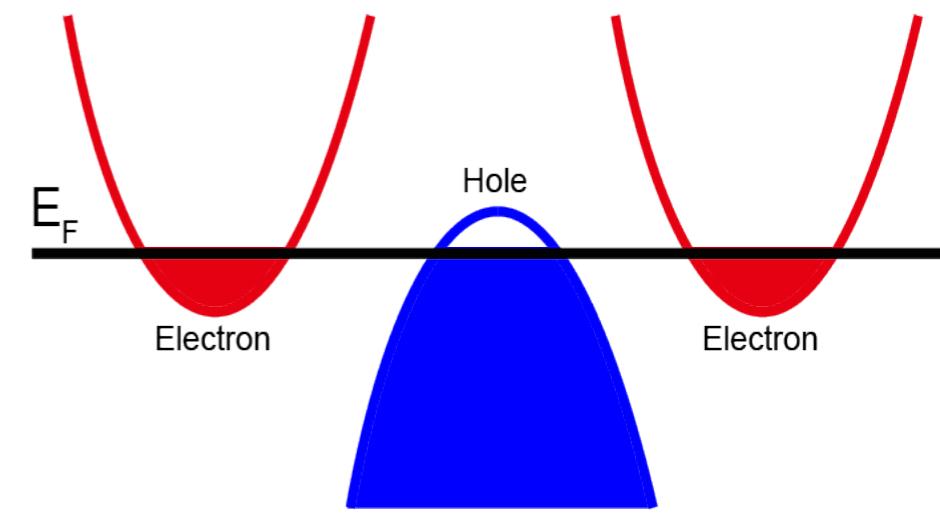
Superconducting $K_xFe_{2-y}Se_2$



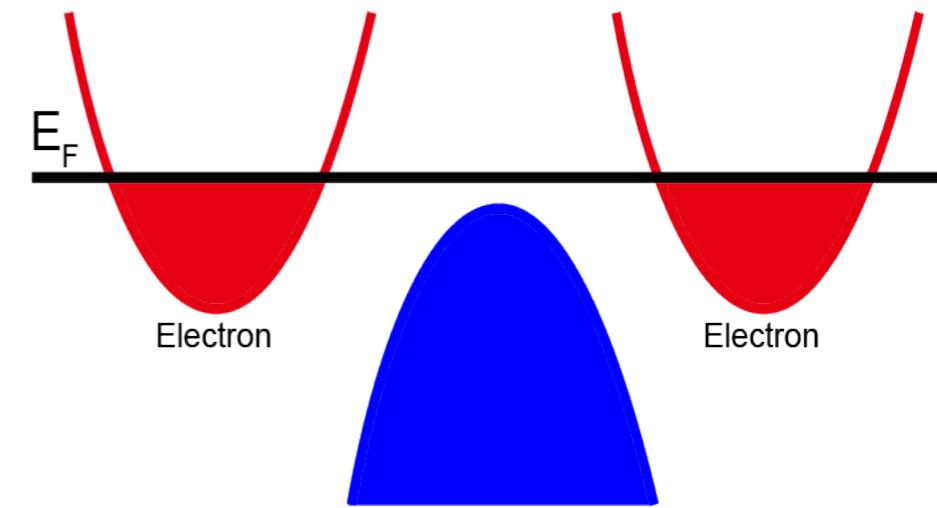
1 ML FeSe/SrTiO₃ thin film



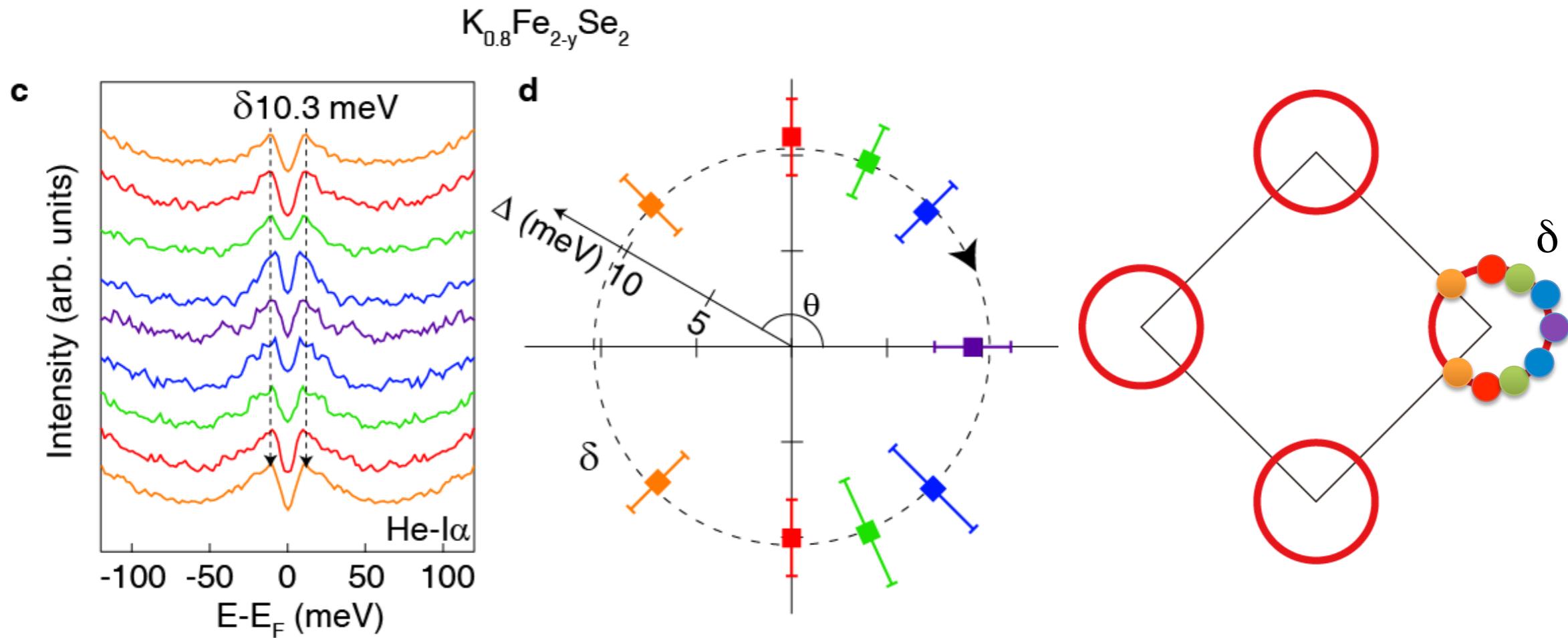
Other iron-based superconductors



$K_xFe_{2-y}Se_2$ and FeSe thin film

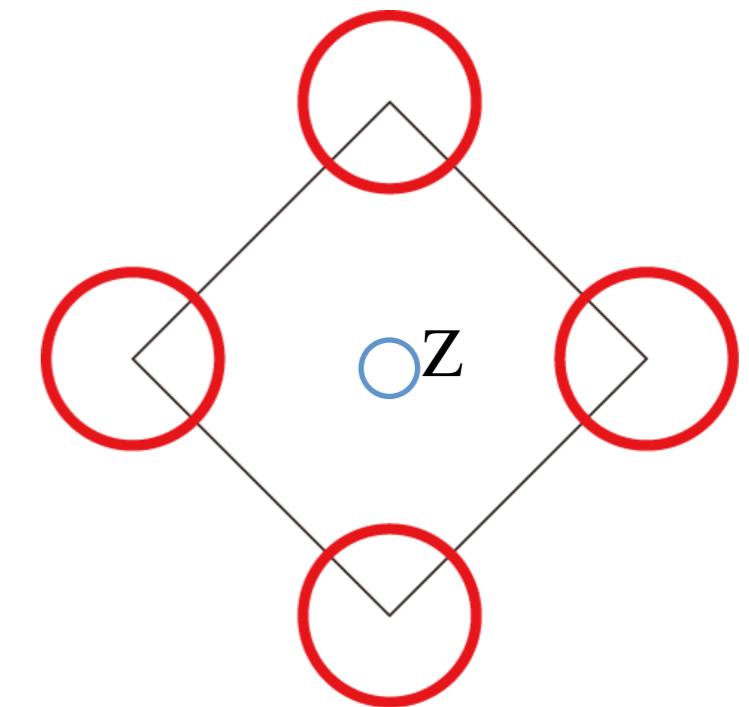
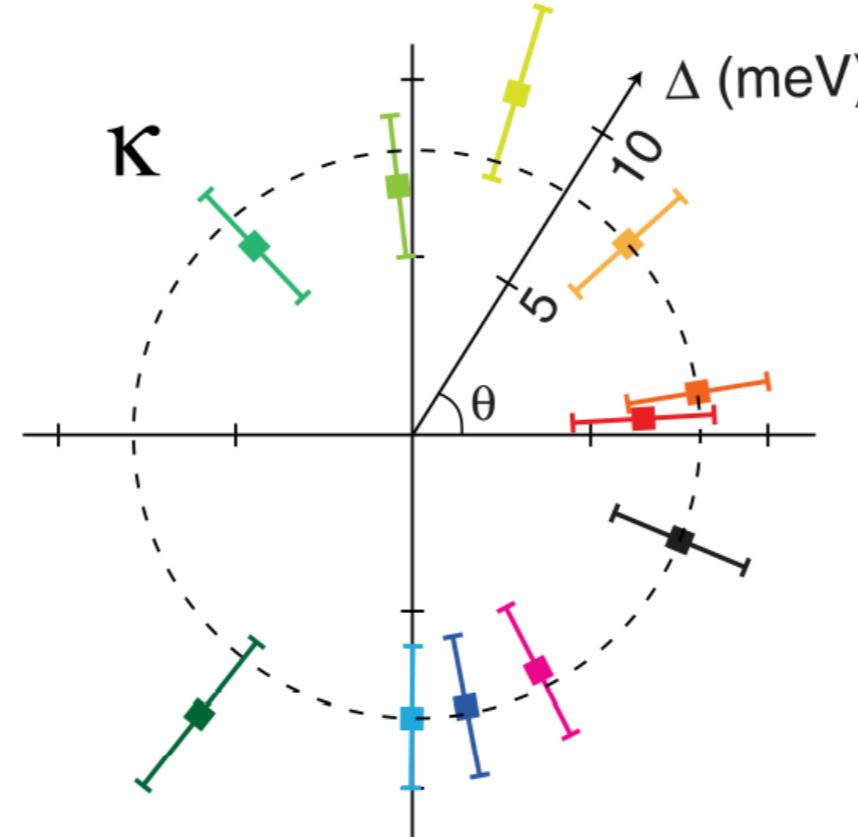
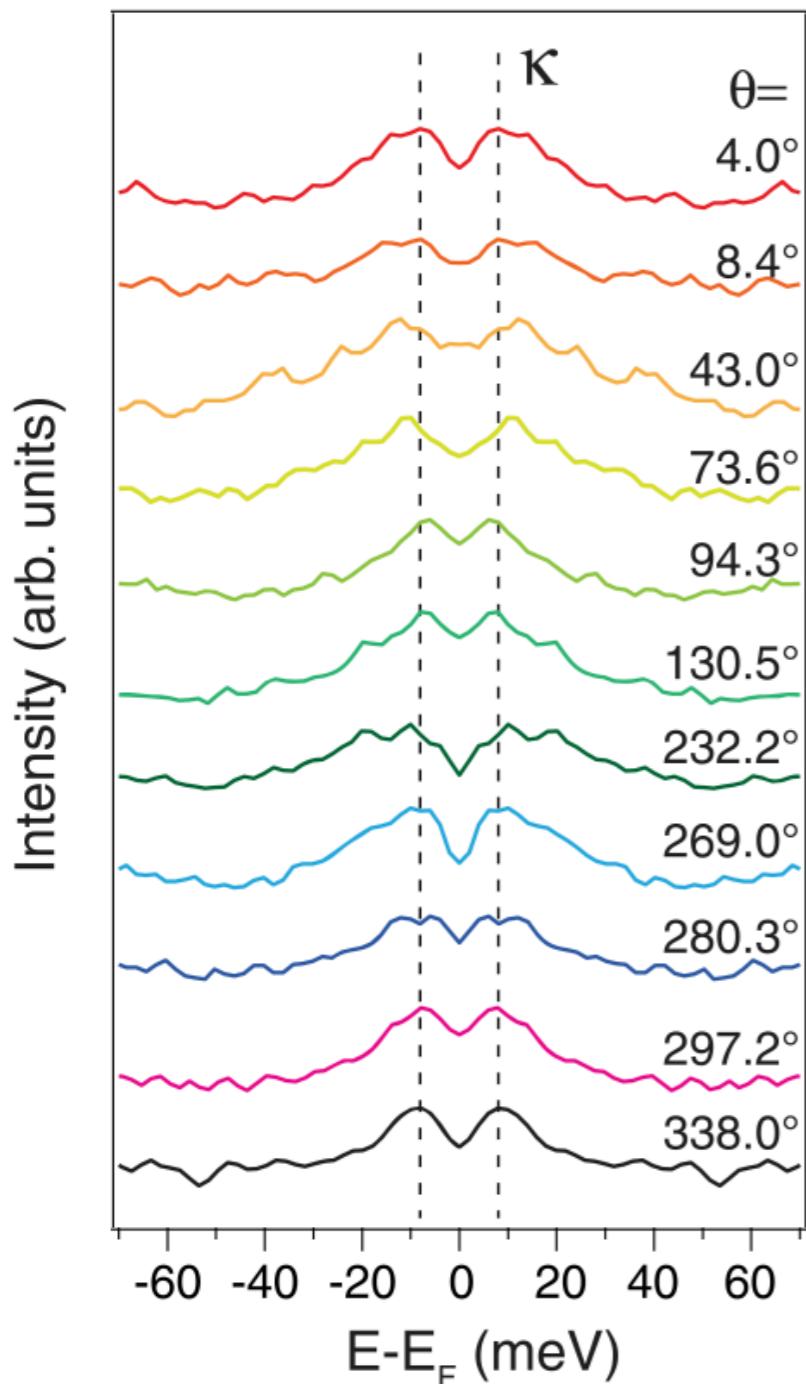


In-plane gap distribution on δ FS of $K_xFe_{2-y}Se_2$



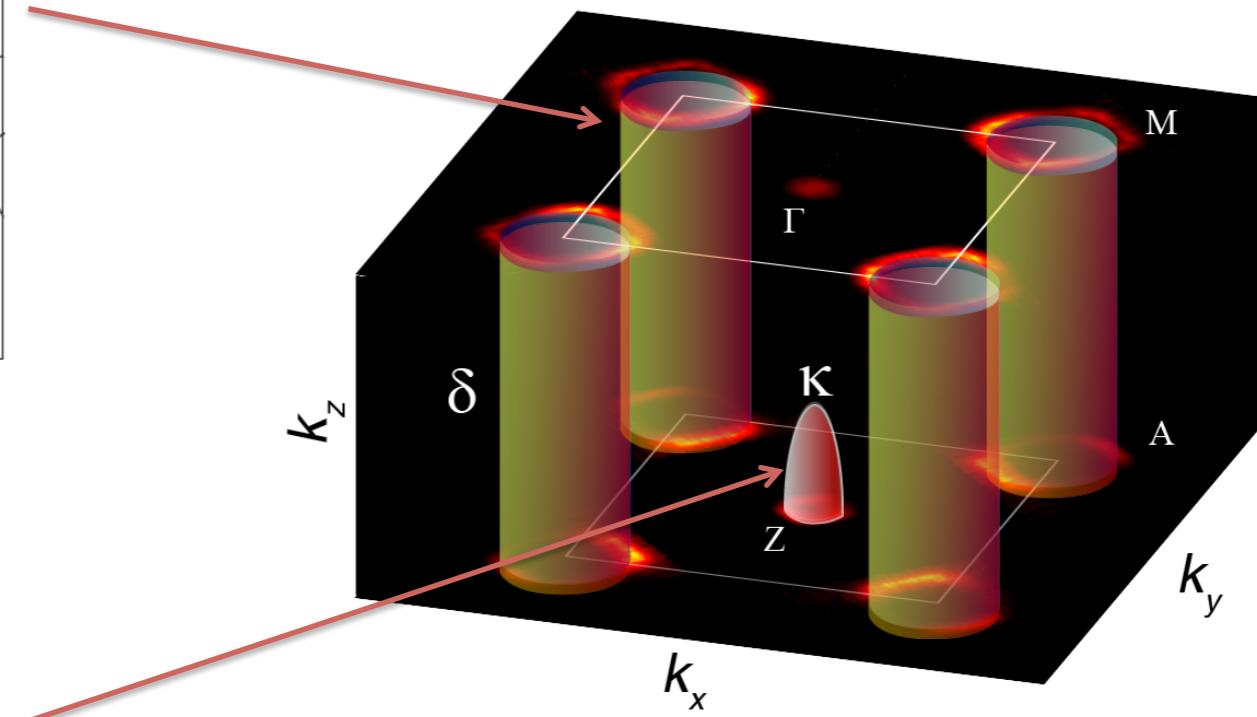
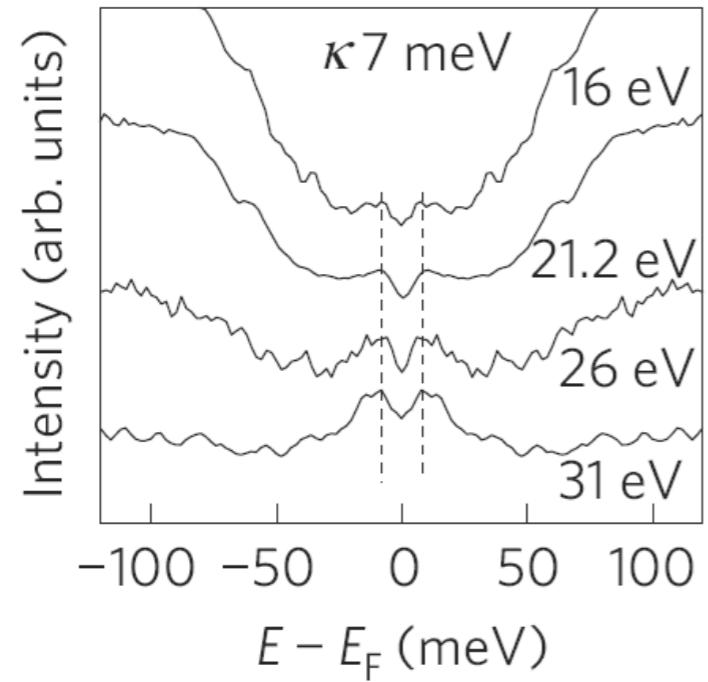
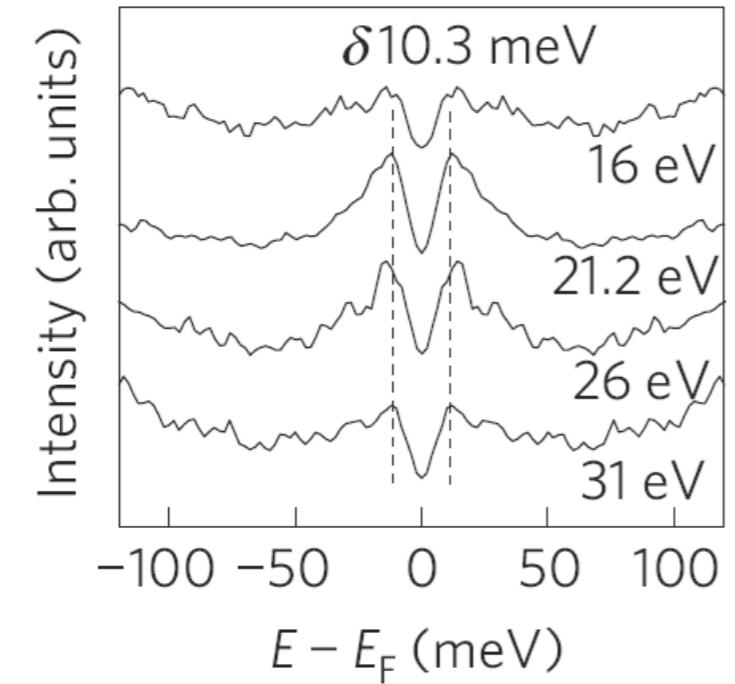
Isotropic nodeless superconducting gap on the corner electron pockets

In-plane gap distribution on κ FS of $K_xFe_{2-y}Se_2$



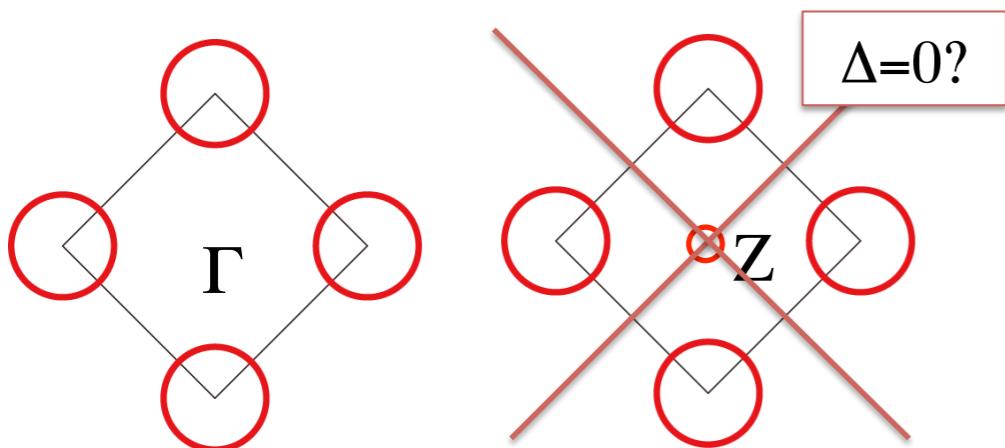
Isotropic nodeless superconducting gap on the center electron pockets.

The gap k_z dependence of $K_xFe_{2-y}Se_2$

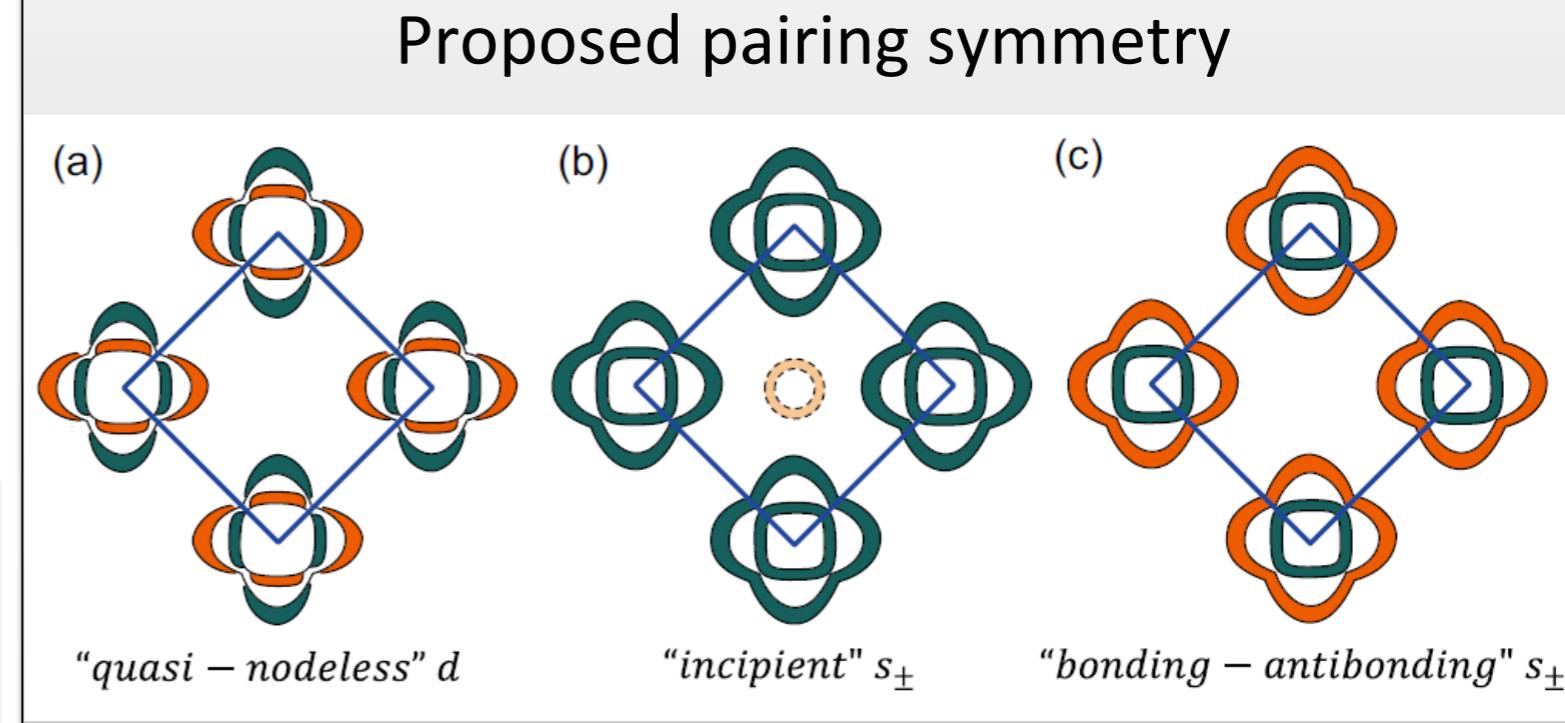


Pairing symmetry puzzle of $K_xFe_{2-y}Se_2$

ARPES: isotropic nodeless superconducting gap in $K_xFe_{2-y}Se_2$



Neutron resonance peak suggests phase change

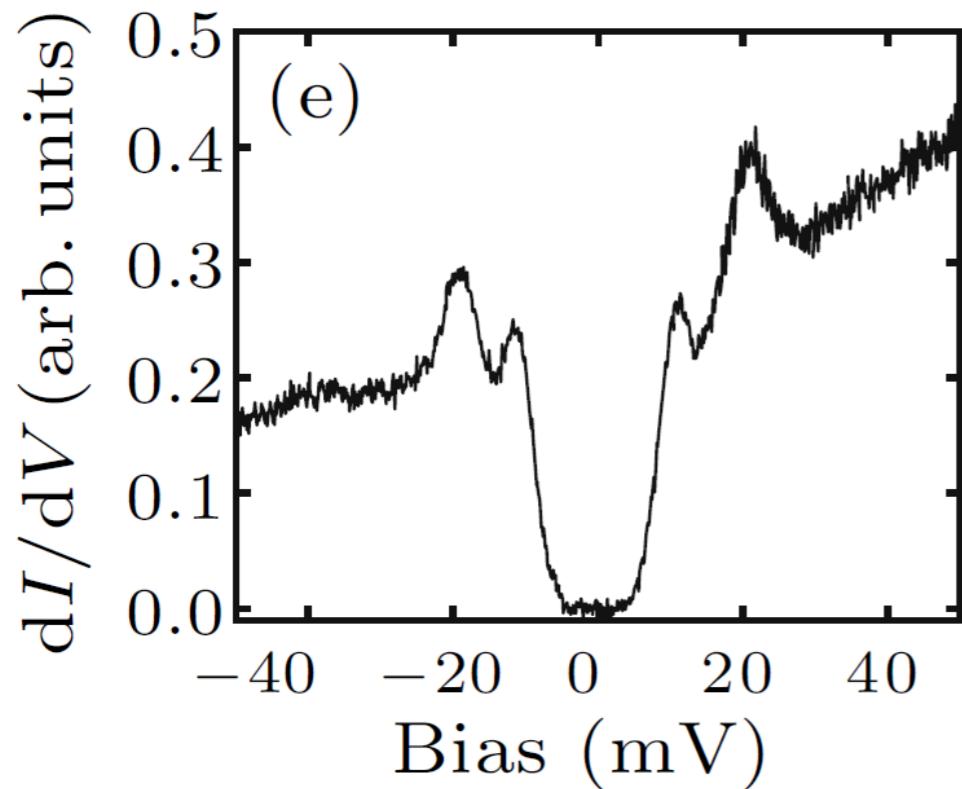


P J Hirschfeld et al., Rep. Prog. Phys. 74 124508 (2011)

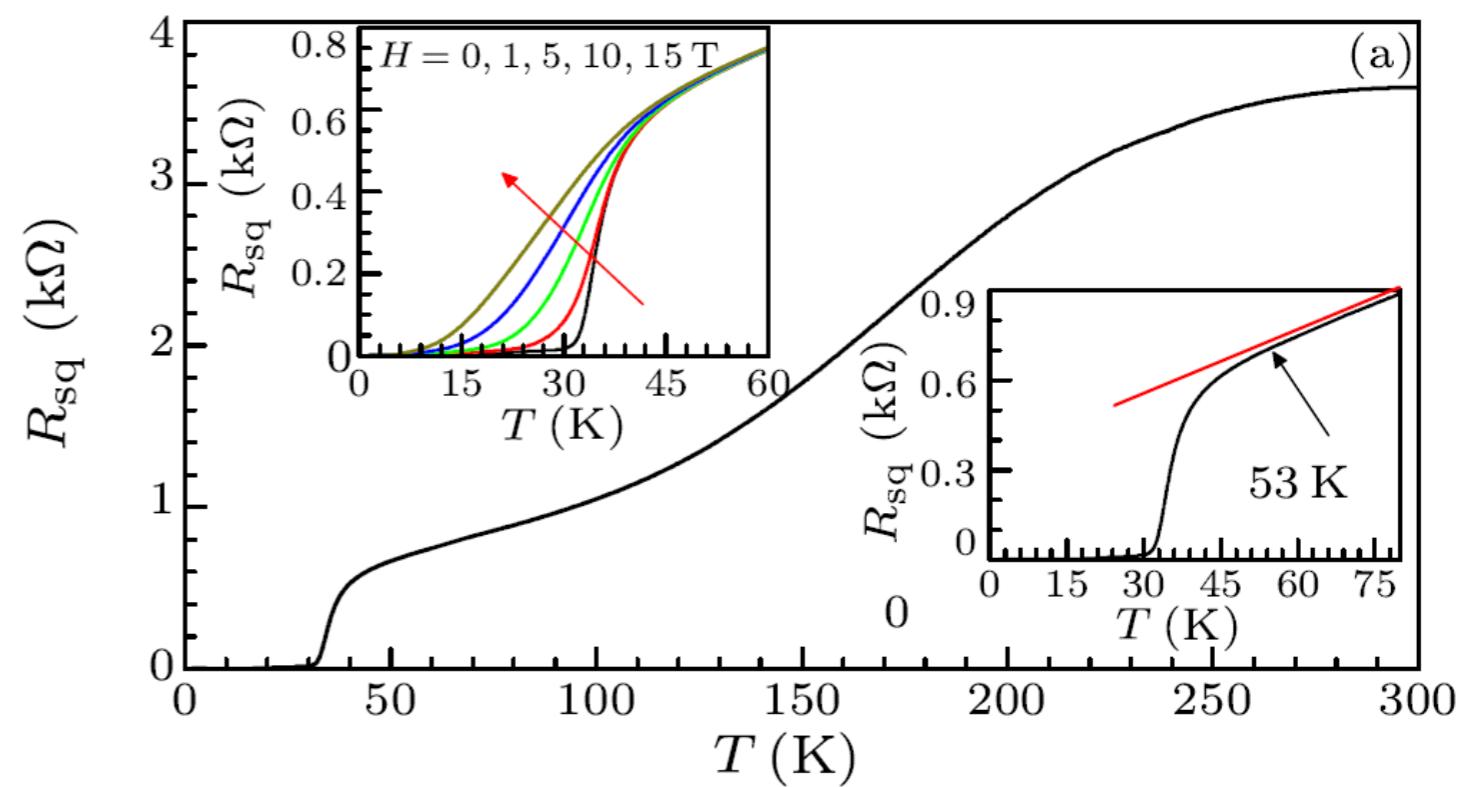
- suggest a s-wave pairing symmetry in $K_xFe_{2-y}Se_2$
- inconsistent with the d-wave pairing symmetry

1ML FeSe/SrTiO₃ thin film

Superconductivity above 77K?



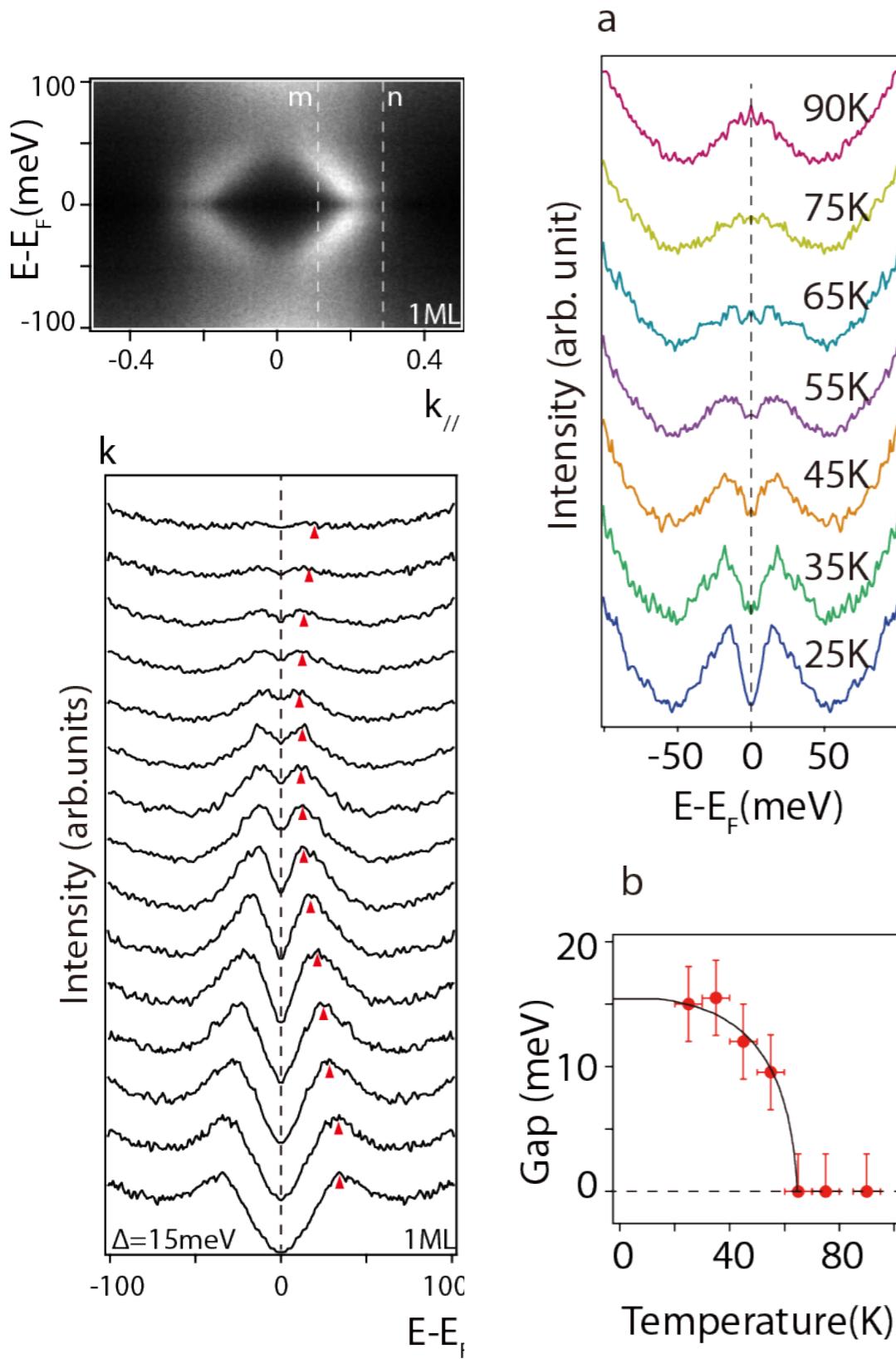
STS of 1ML FeSe ($\Delta \approx 20.1 \text{ meV}$)



Transport Measurement of 5ML FeSe

KT transition or measurement issue?
Wang Q.Y. *et al.* Chin. Phys. Lett. 29, 037402 (2012)

Gap distribution in 1ML FeSe/STO thin film

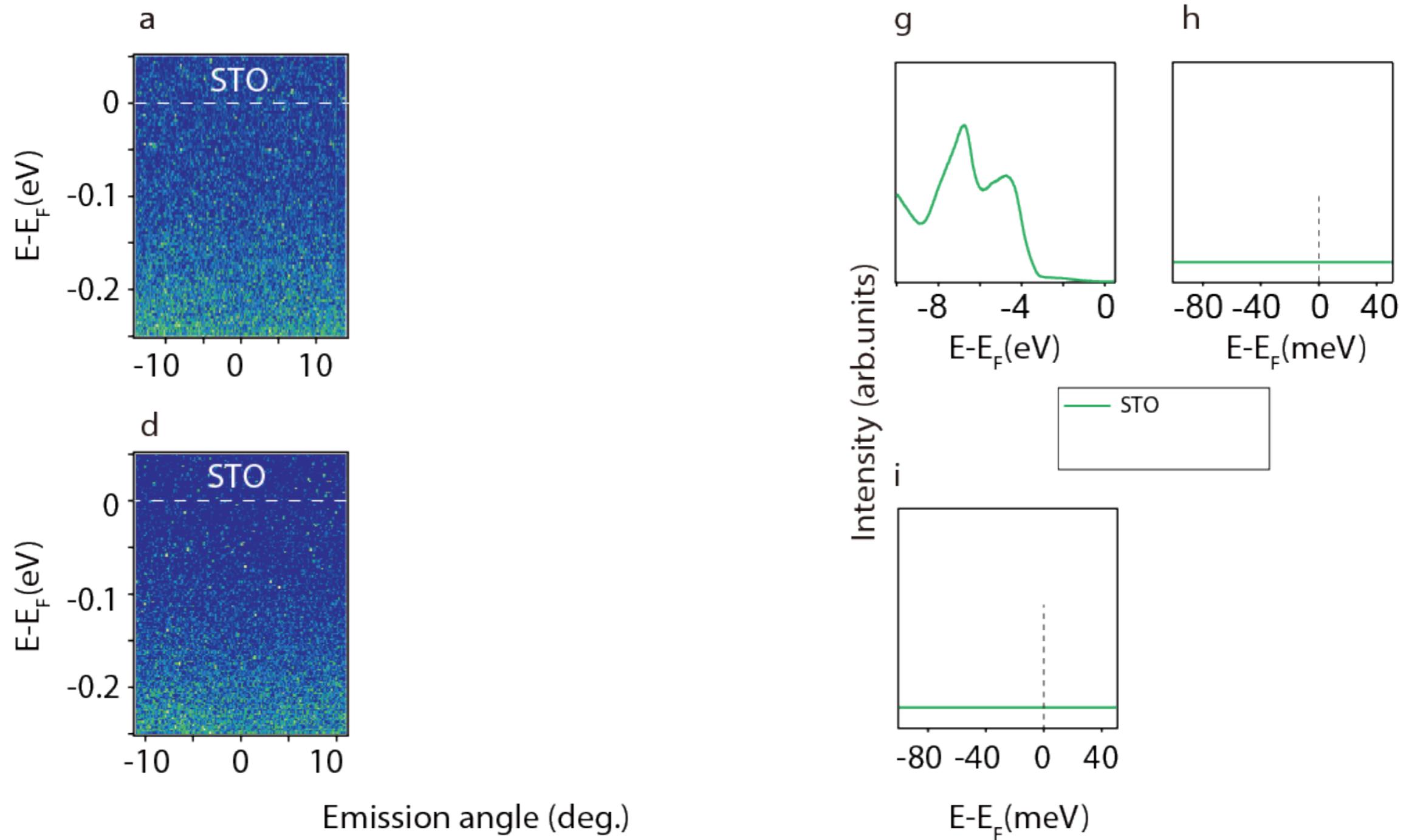


D. Liu XJ Zhou et al., Nat Commun 3, 931 (2012).

Isotropic nodeless superconducting gap in FeSe film

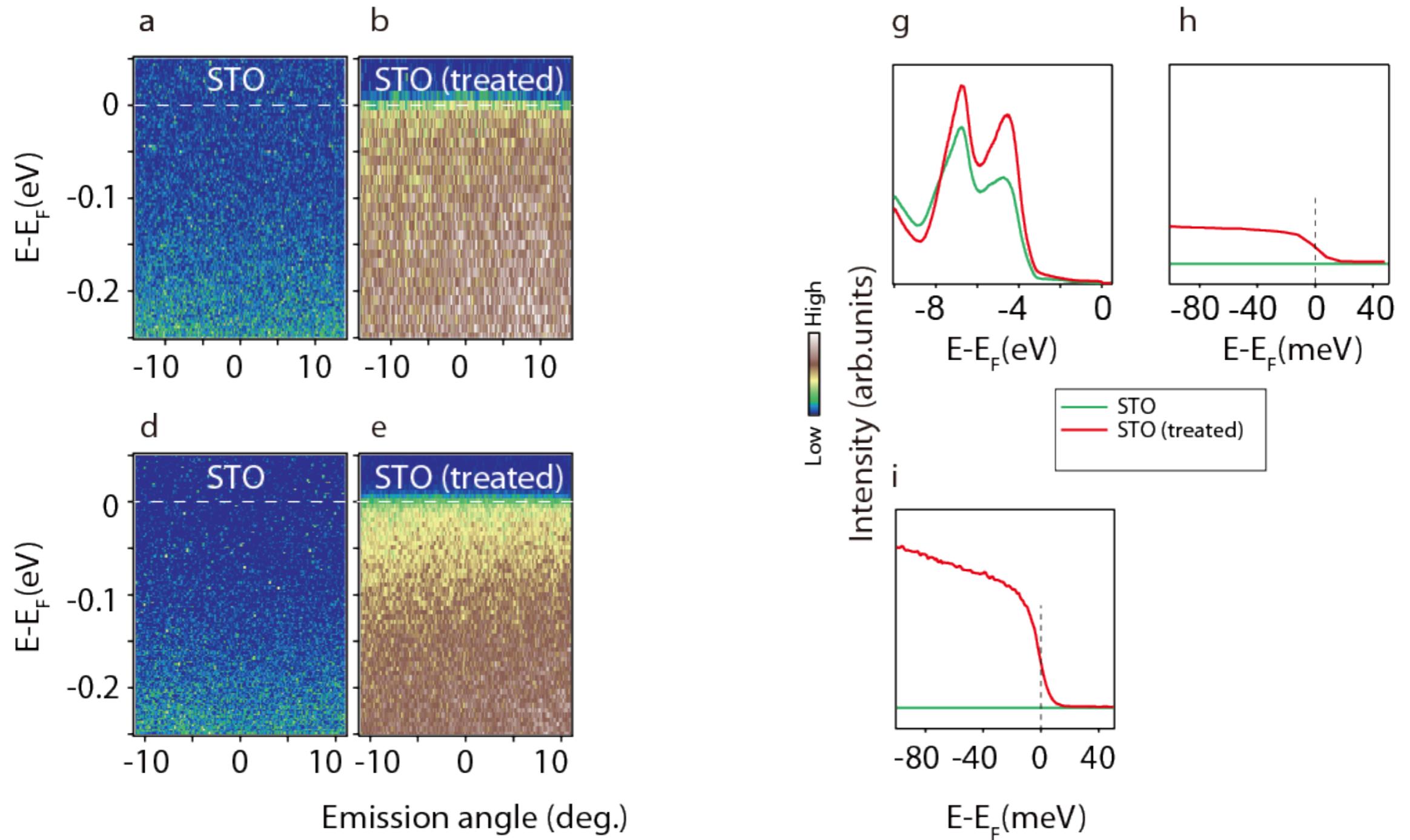
s-wave gap symmetry

Where are the extra electrons in 1ML FeSe from?



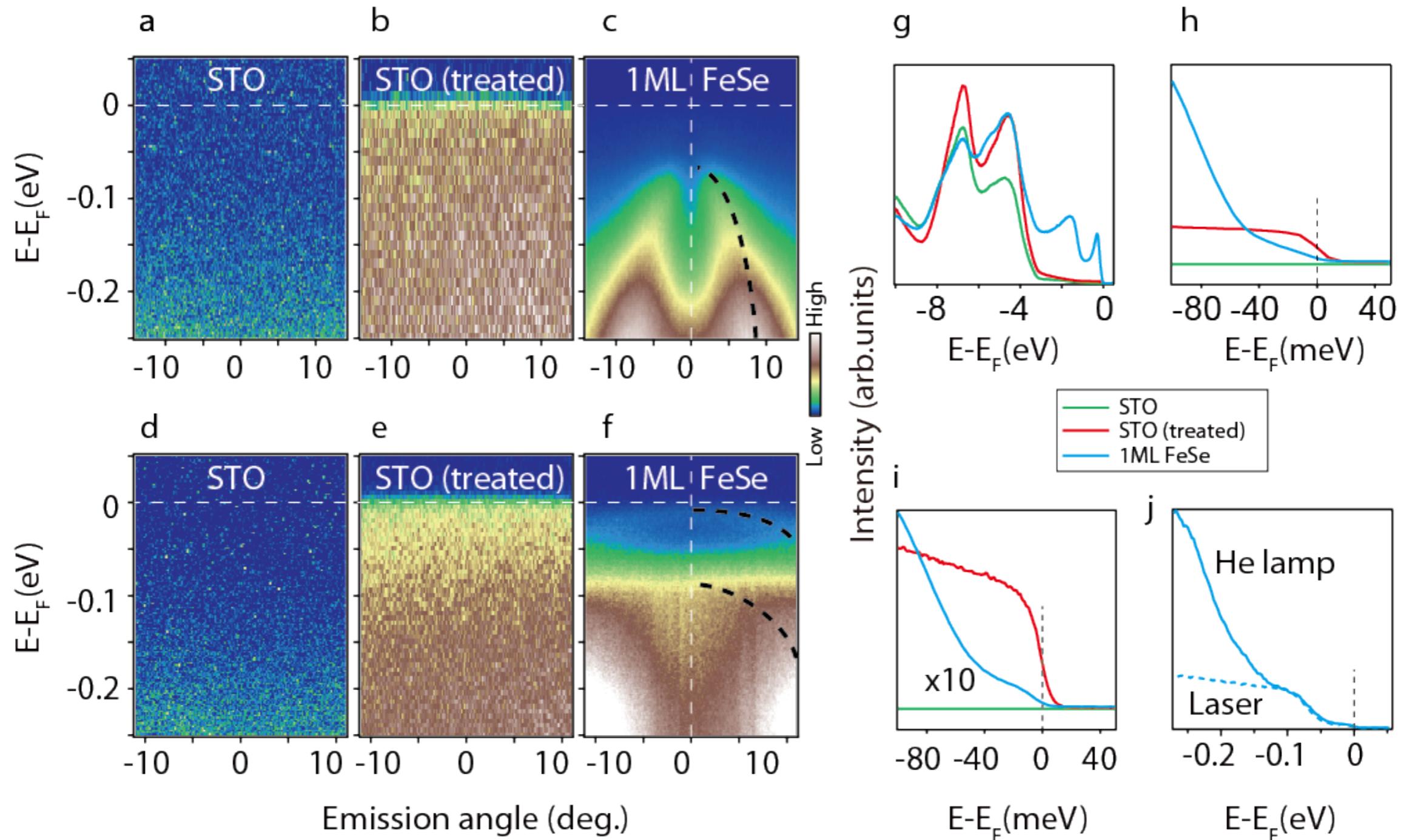
- The STO substrate presents insulator-like behavior after degas

Where are the extra electrons in 1ML FeSe from?



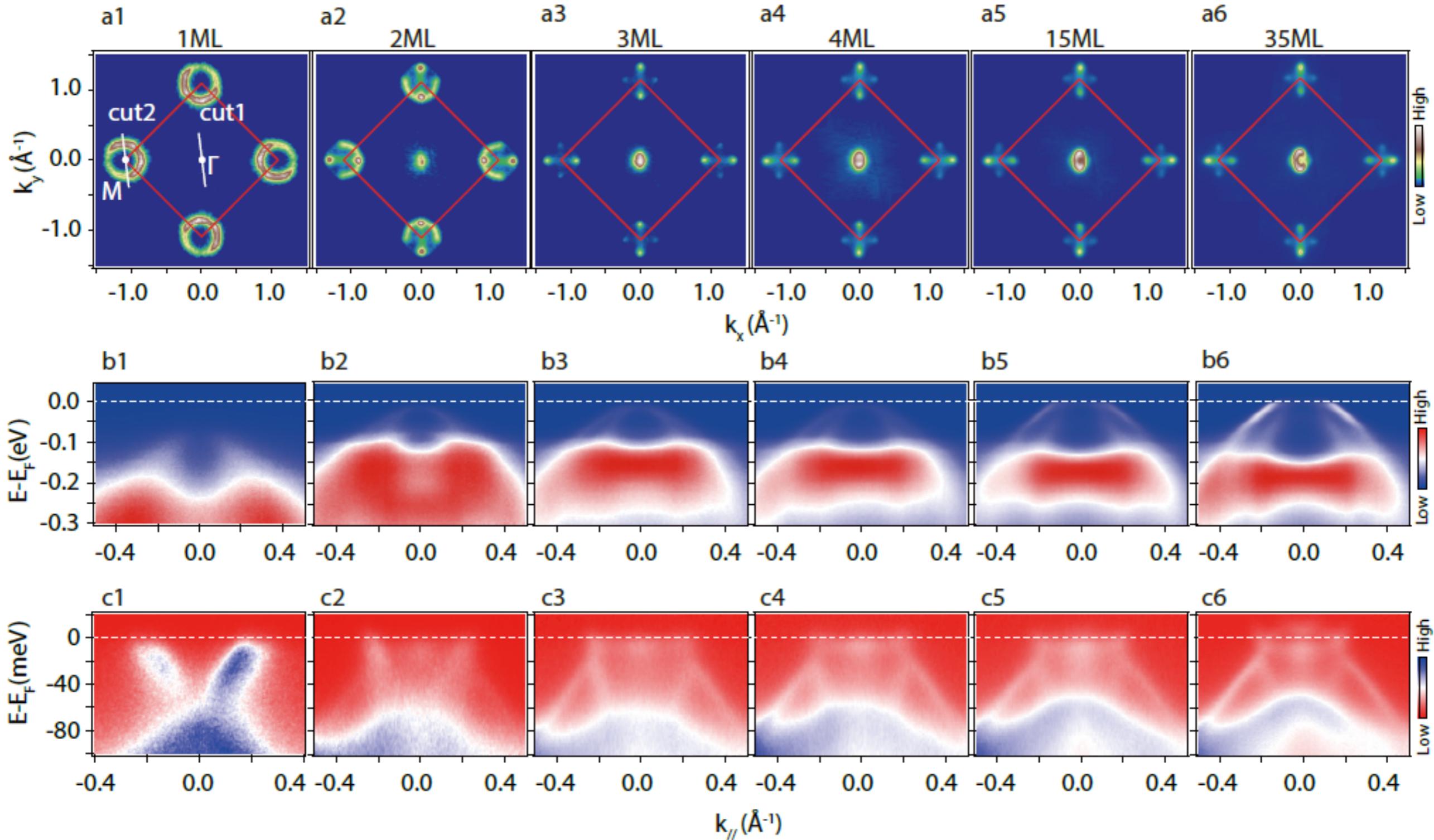
- The STO substrate presents insulator-like behavior after degas, **and metallic conductivity appears after thermo-treatment at 950 °C under Se flux.**

Where are the extra electrons in 1ML FeSe from?



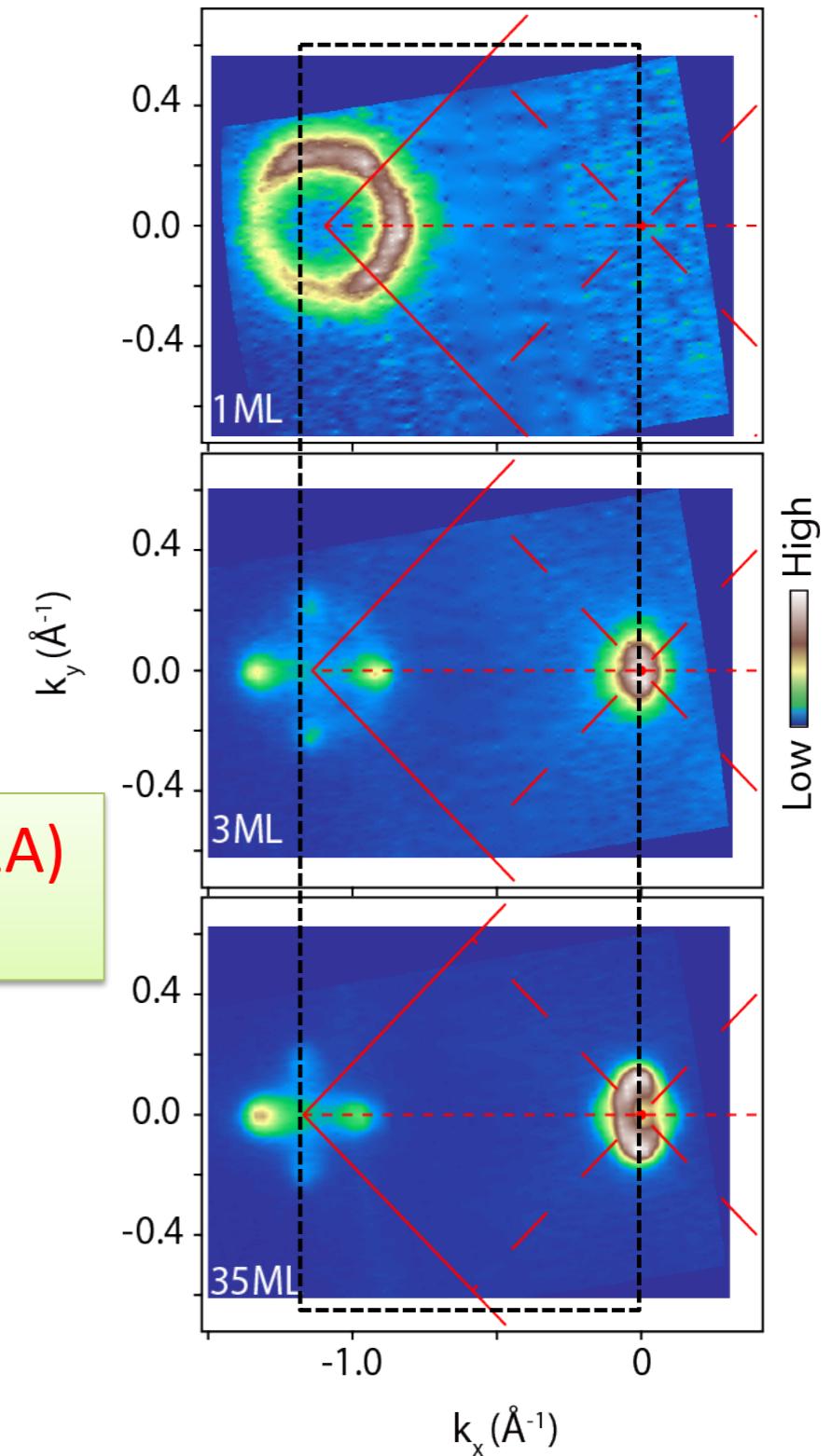
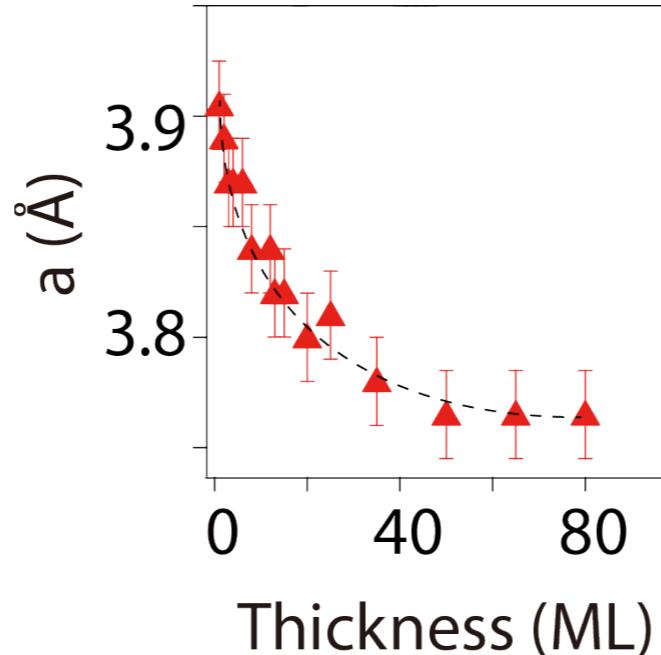
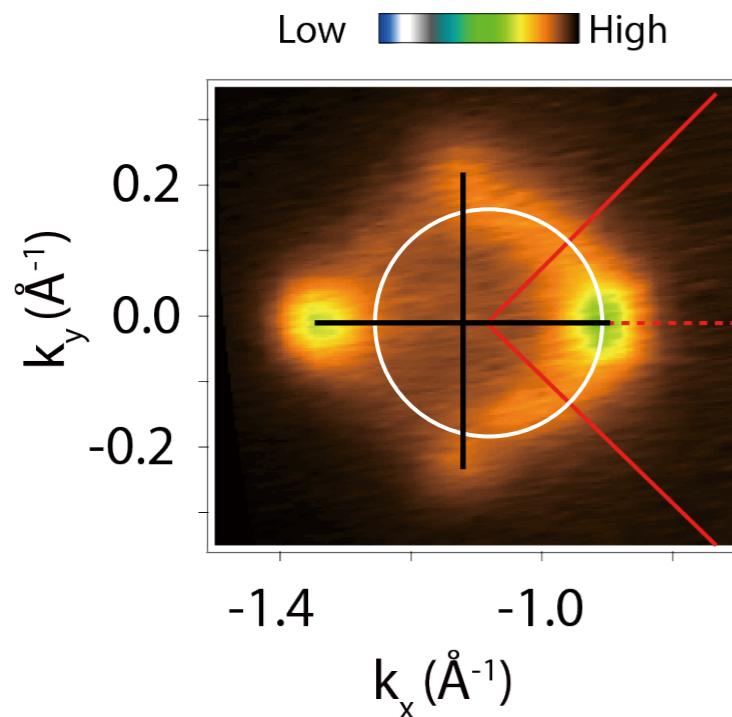
- The STO substrate presents insulator-like behavior after degas, and metallic conductivity appears after thermo-treatment at 950 °C under Se flux.
- After the 1ML FeSe was deposited, the electrons are transferred to the FeSe layer, and thus are responsible for the electron doping in 1ML FeSe.

Electronic Structure Evolution

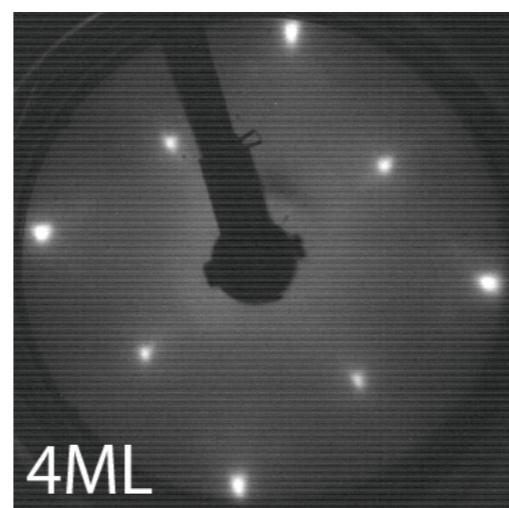
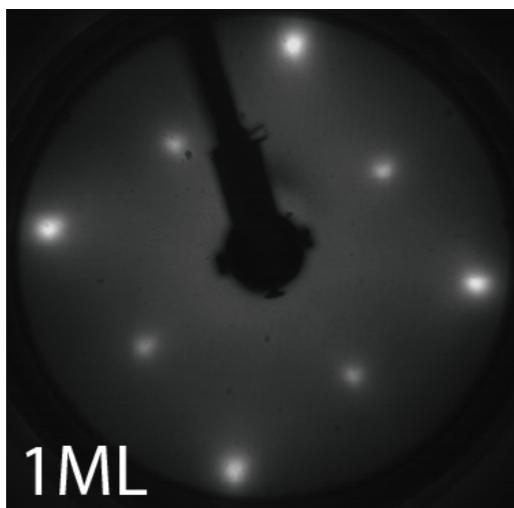


Interfacial layer: 0.12e- excess electrons per Fe
Other layers: charge neutral (within 0.01e-/Fe accuracy)

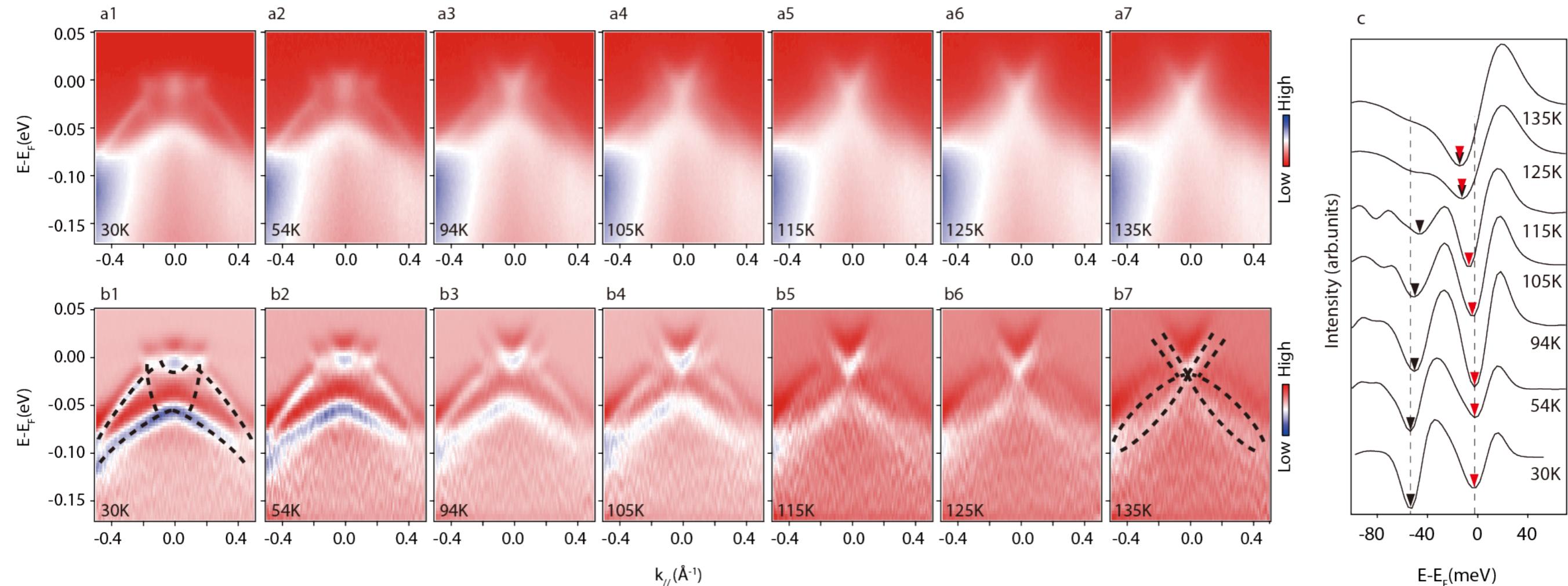
Thickness Dependence of the Lattice Constant



The in-plane lattice is relaxed from the STO (3.91\text{\AA}) to the bulk FeSe value (3.76\text{\AA}) in thick films

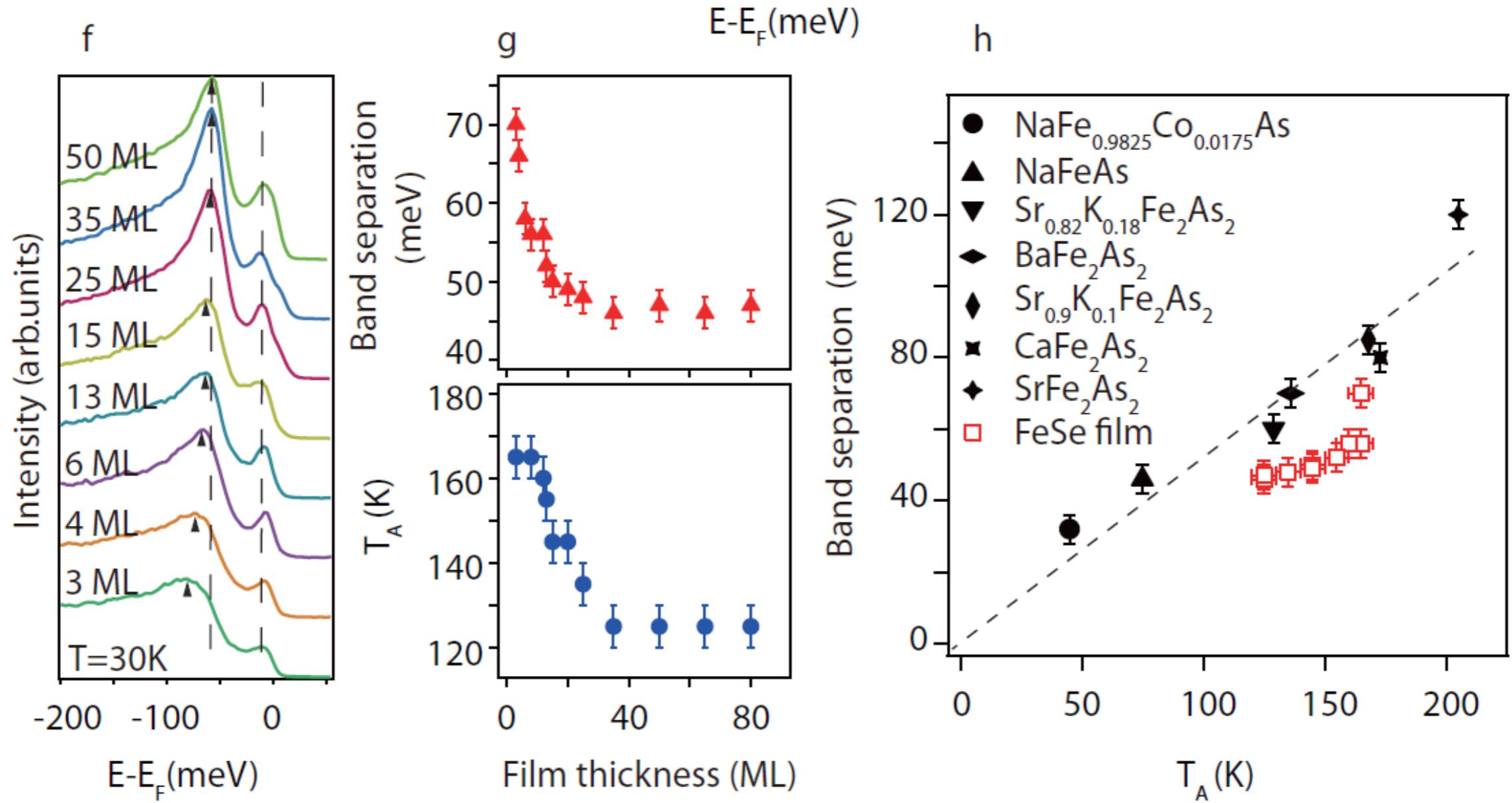


SDW in Multi-Layer FeSe (50ML)



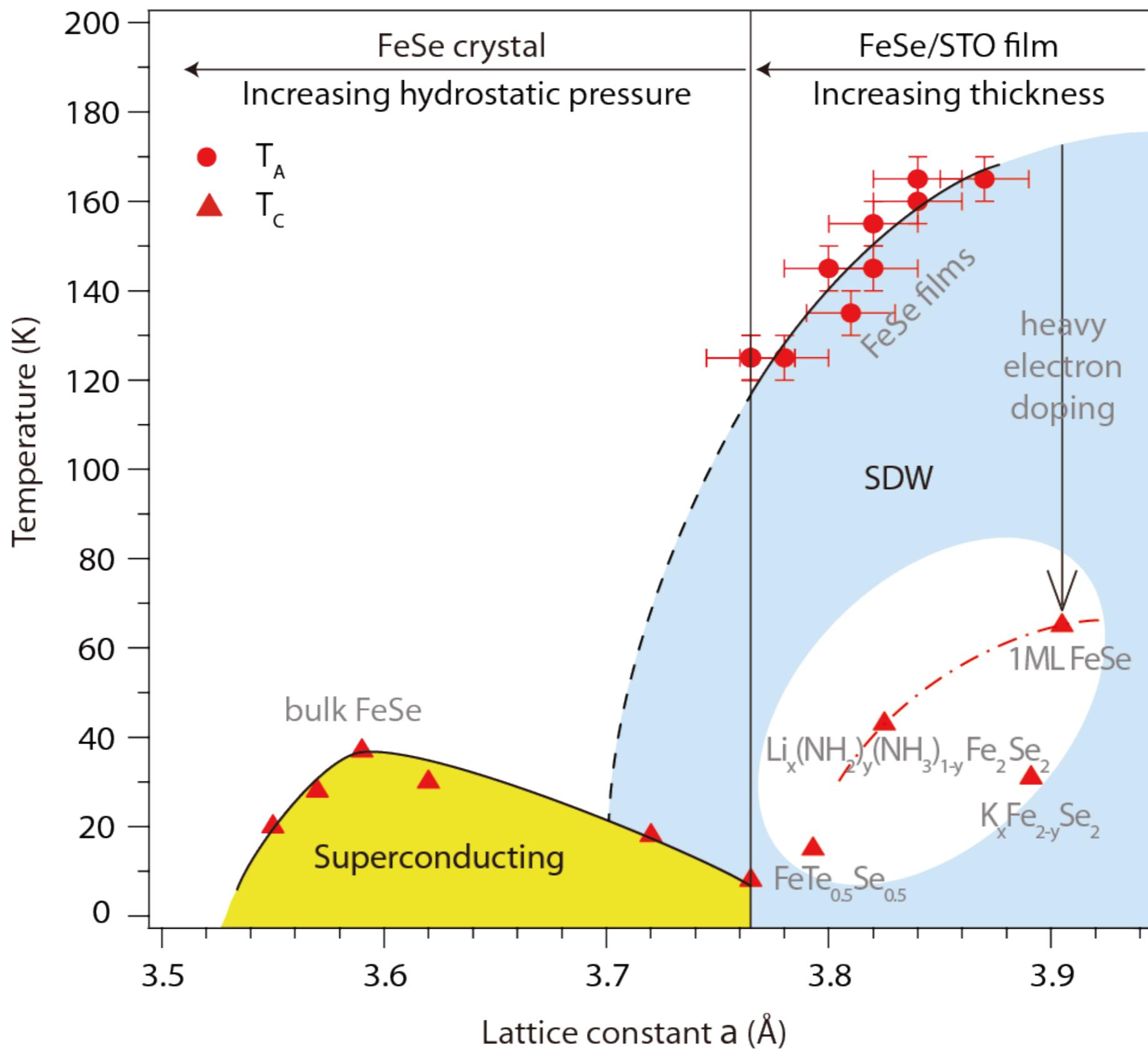
With increasing temperature, the two separated bands gradually become degenerate above 125K.

Strain-Dependent SDW

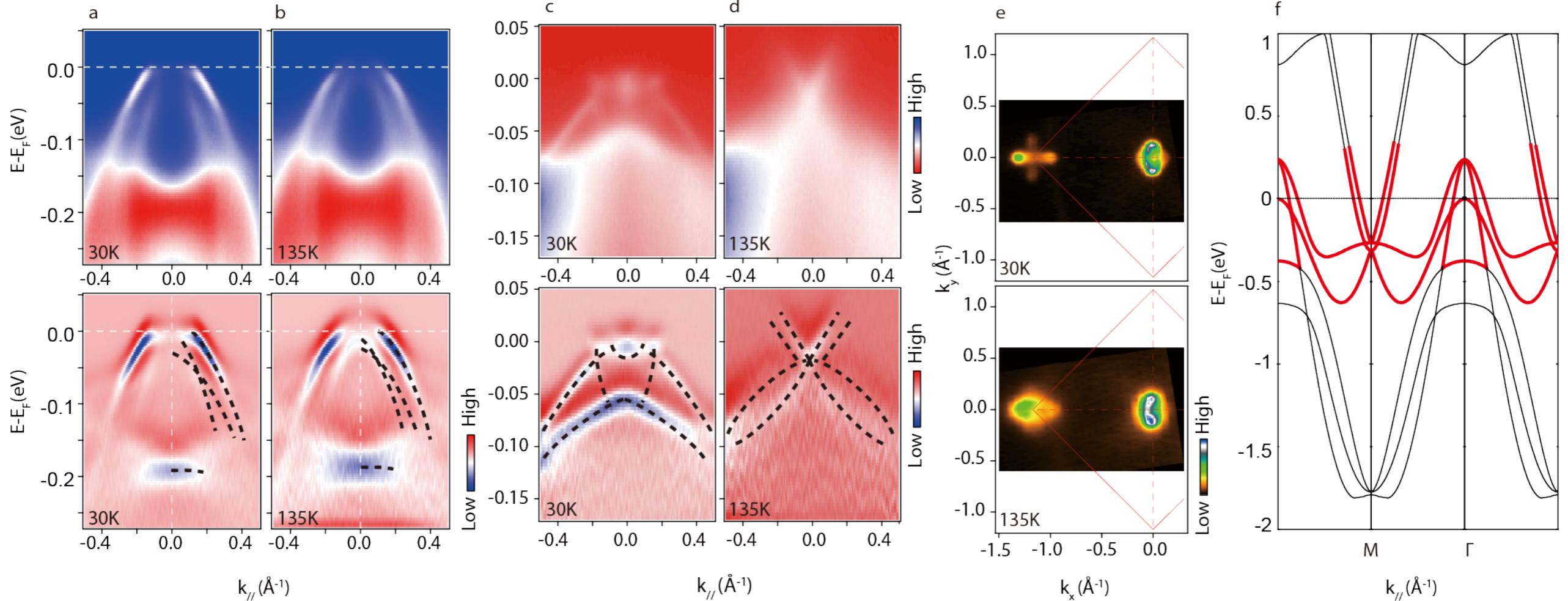


- The band separation and phase transition temperature decreases with increasing film thickness.
- Our calc. shows enhanced lattice size increases J_2 , and prefers the collinear AFM.

Phase Diagram



FeSe (50ML, close to bulk)

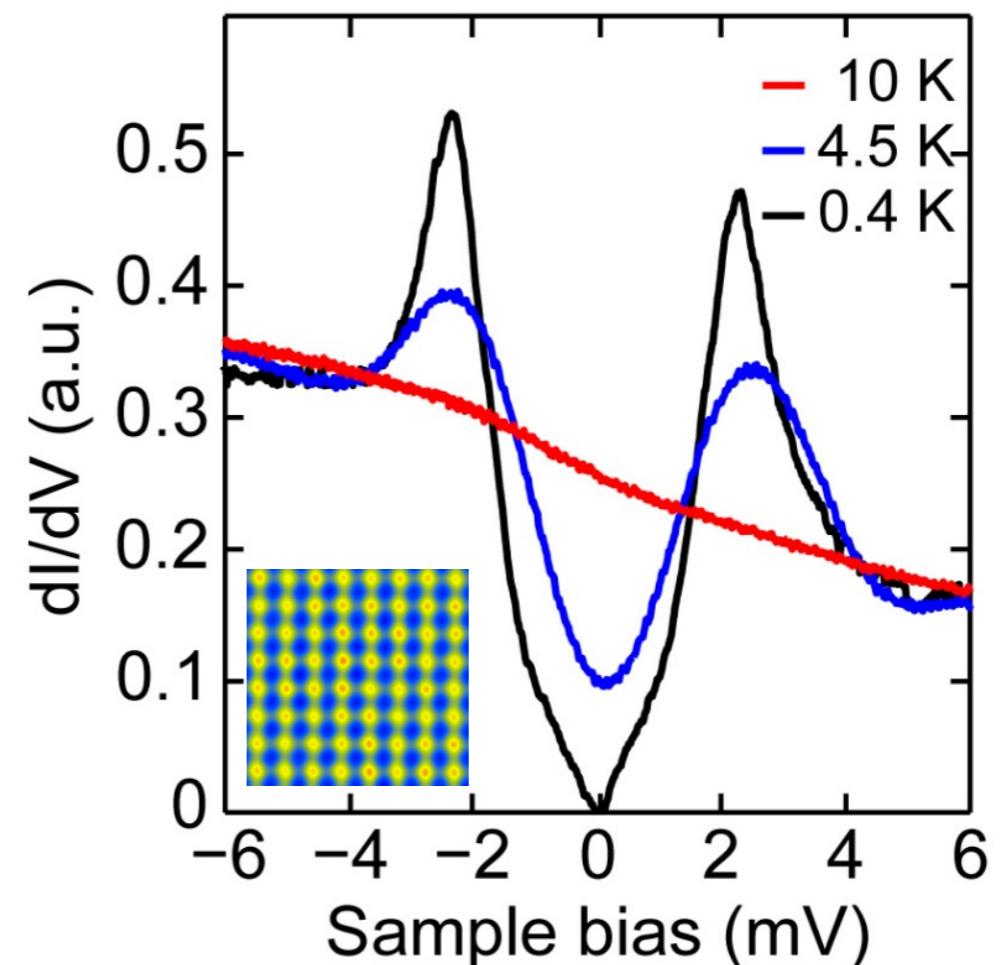
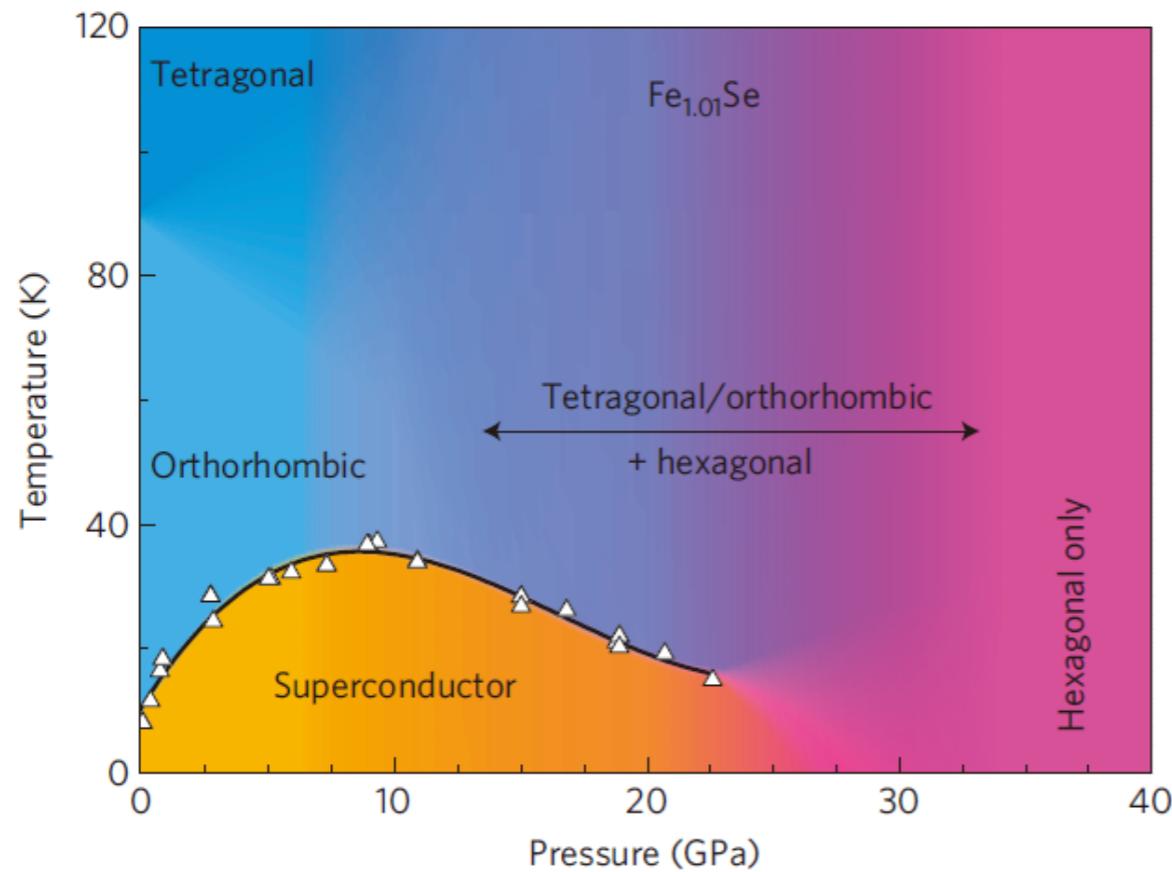


- SDW (at least strong fluctuation) exists in bulk FeSe, as predicted.
- Explains the nodes measured by Qikun Xue et al. the ortho-tetra transition.
- The electronic structure of 50ML FeSe agrees well with the band calculation*, and represent the bulk electronic structure of FeSe.

* Ma, F. *et al. Phys. Rev. Lett* 102, 177003

FeSe

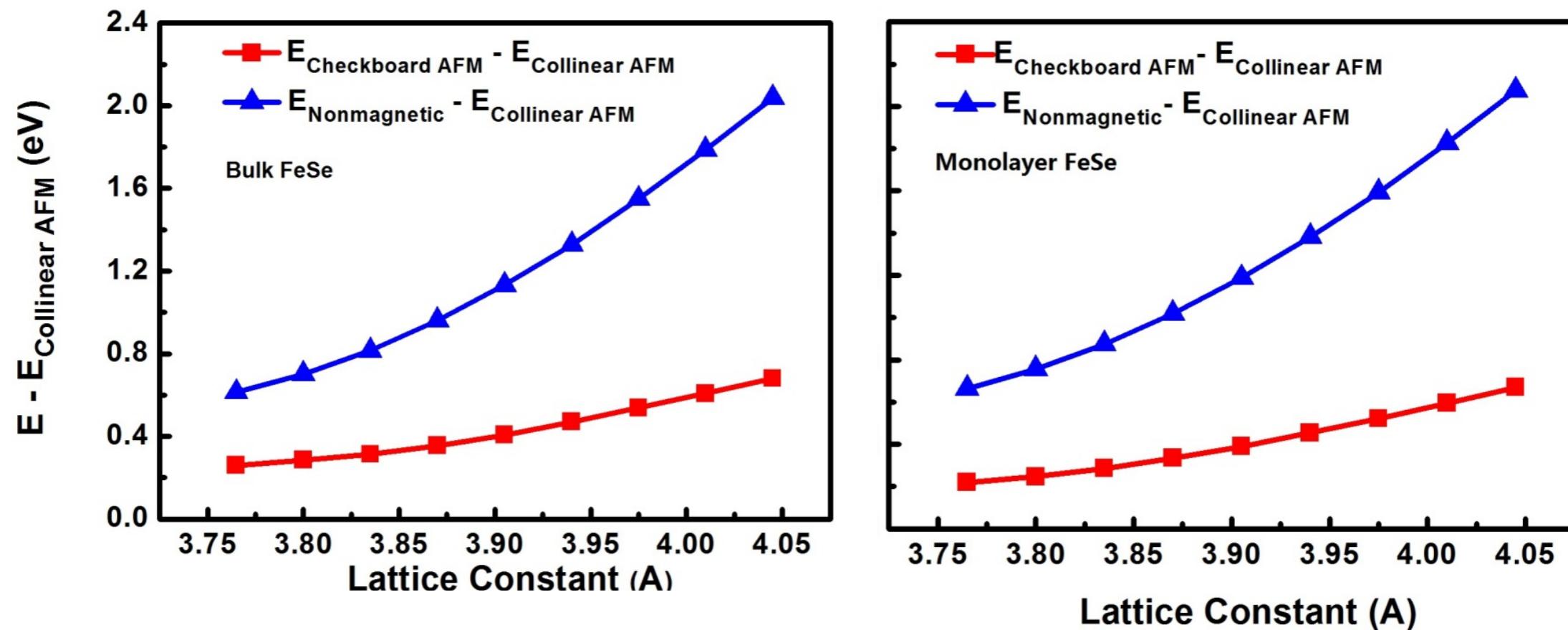
- Superconducting $T_c=8\text{K}$, & 37K under 8.9 GPa .
- LDA predicts a CAF ground state
- 110K anomaly in ultrafast optics
- Ortho-tetra transition



Medvedev, S., et al. (2009). Nature Materials 8

C. L. Song, Q. K. Xue et al. Science, 2011

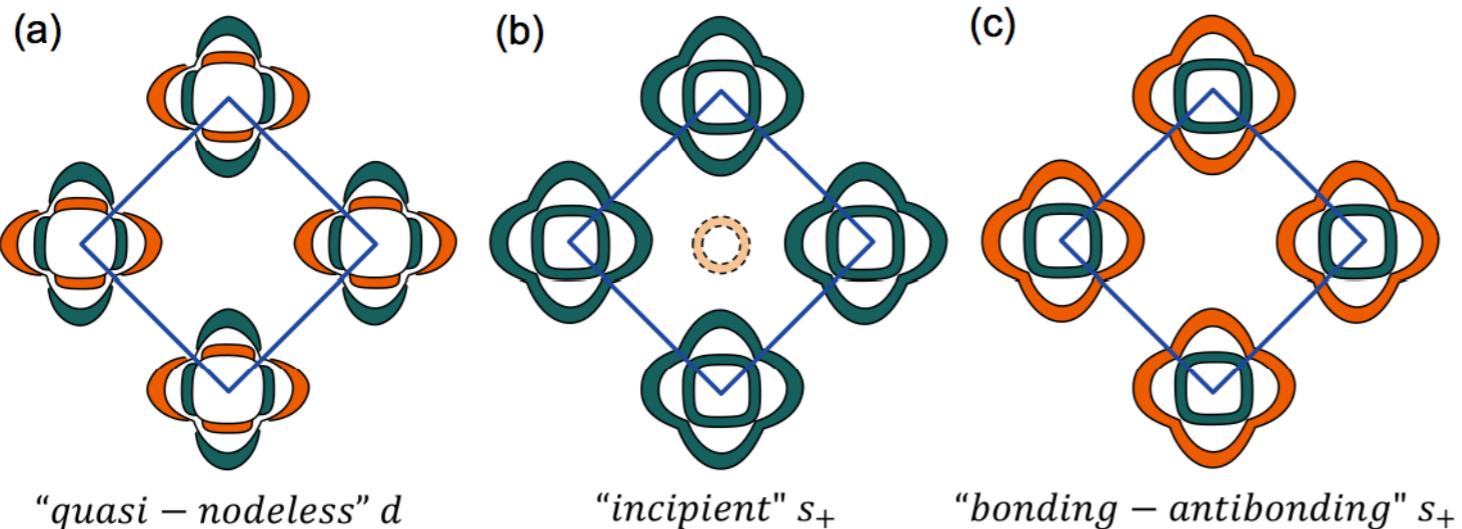
LDA+GGA calculations explains the evolution of SDW



- enhanced lattice → enhanced Fe-Se-Fe superexchange
→ enhanced SDW .
- Oxygen vacancies induce doping → suppress SDW
- Enhanced J → T_c enhancement?

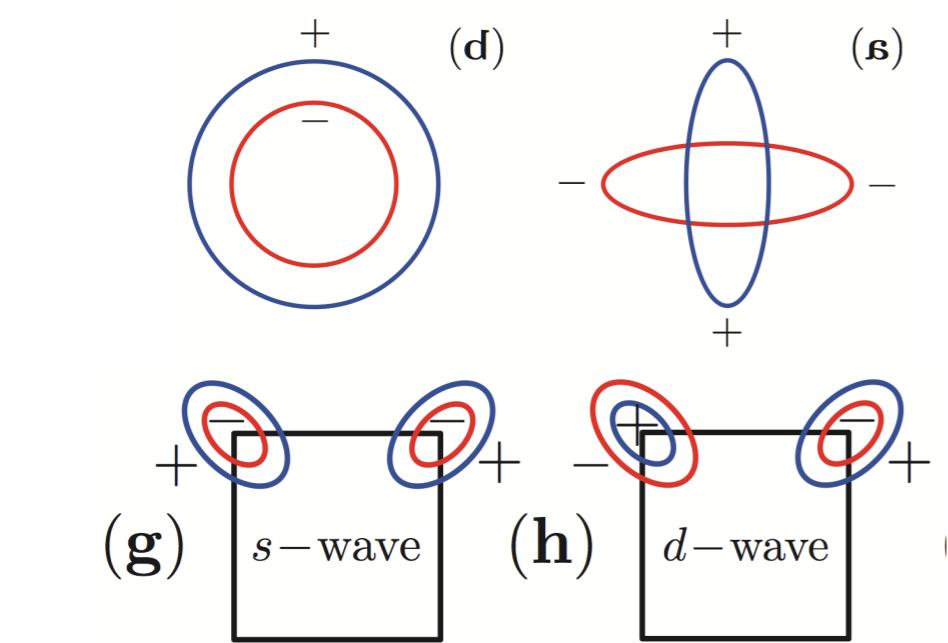
Scenarios on the table

A good scenario should explain all K_xFe₂Se₂, FeSe/STO, and FeSe/STO/KTO

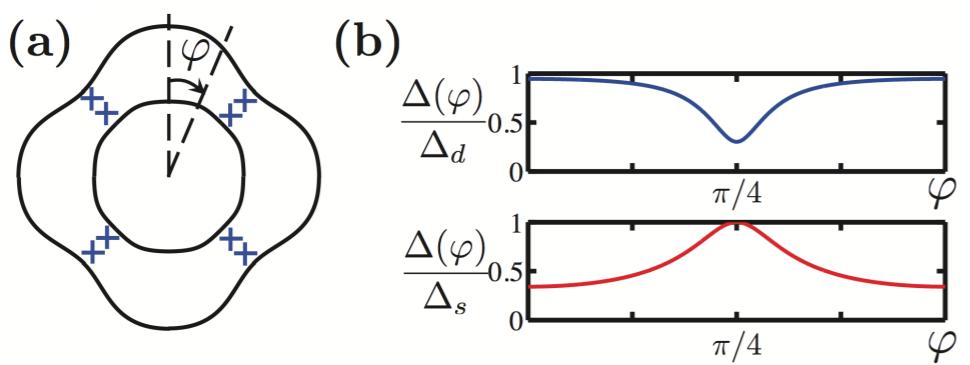
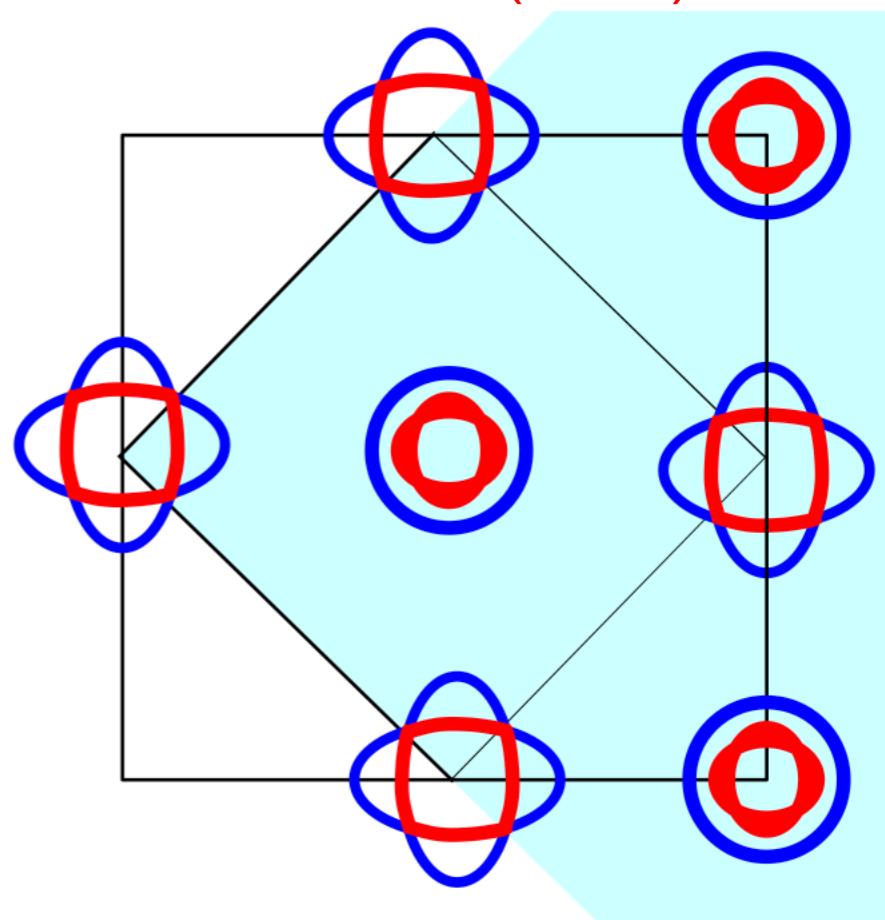


Hirschfeld et al Rep. Prog. Phys.
74 (2011) 124508

Nodes?
Hybridization?



Odd Parity Superconducting State
Hu et al. (2013)



Nodes in k_z direction

Khodas & Chubukov, PRL 108, 247003 (2012).

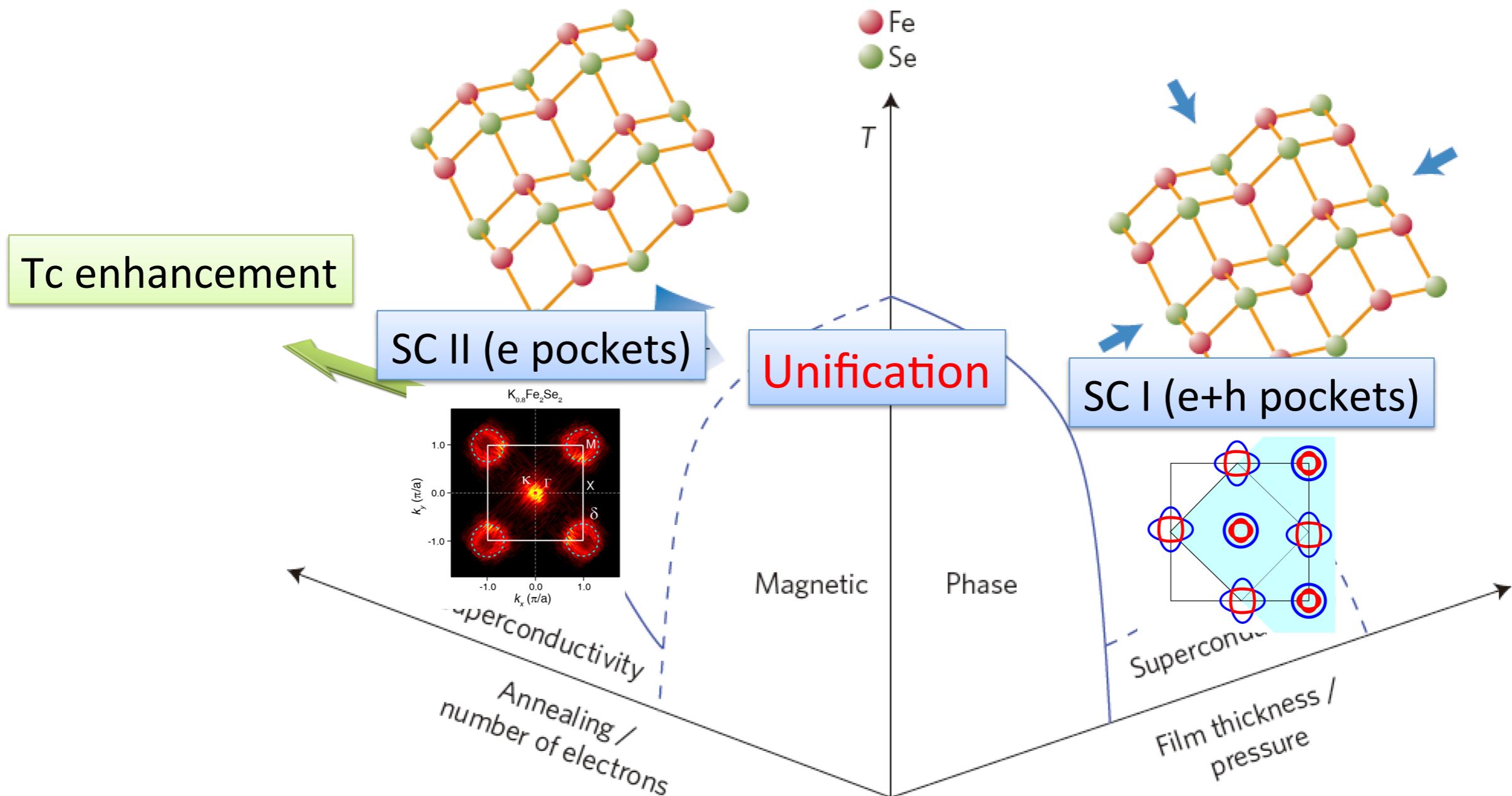
What governs T_c for Type-II Fe-HTS's

Fermi surface topology may not be very important, as it changes a lot in FeSe/STO/KTO, but T_c only changes slightly.

- Reduce disorder with ammonia intercalation (wet method, more moderate growth) gives higher T_c
- Similarly, less impurity scattering for FeSe film than for K_xFe₂Se₂ with heavy phase separation and disorder
- Increase lattice constant (compared with bulk FeSe) → increase J
- proximity to the CAF phase (the block AFM may not be relevant)
- then kill the order by doping (K, or oxygen vacancy)

Fewer atoms, more information

Sergey Borisenko, *Nature Materials* (2013)



1. The s-wave pairing symmetry appears ubiquitous
2. Two types of FeHTS's are in the two sides of the collinear SDW phase.

Summary: What governs Tc for all Fe-HTS's ?

- 1. Local pairing (large Q and E range), high energy spin fluctuation matters, not the zero frequency ones**
 - Both types are next to the same CAF
 - Fermiology vary significantly, and the role of Fermiology may not be that significant, although nesting helps somewhat, but not critically
 - Large J helps
 - Large local moment suggested by neutron even at high T
- 2. Enhance the instability (J), but not statically ordered (killing it by doping etc.) → in the vicinity of a QCP: not at it, but certainly not far.**
- 3. Shallow, flat band provides large phase space for SC (also related to strong correlation)**
- 4. Minimized impurity scattering matters!**

Outlook

- Further T_c enhancement in thin films, and prove it with in situ transport measure. (enlarge lattice in pnictides?)
- Pairing symmetry or order parameter phase puzzle (smoking gun evidence? η -pairing, s \pm , s $++$, d-wave)
- More experiments, tuning K_xFe₂Se₂, FeSe with doping and strain
- Spin fluctuation as pairing glue? Combine ARPES and INS, searching for effects that matter to superconductivity
- Quantify impurity effects